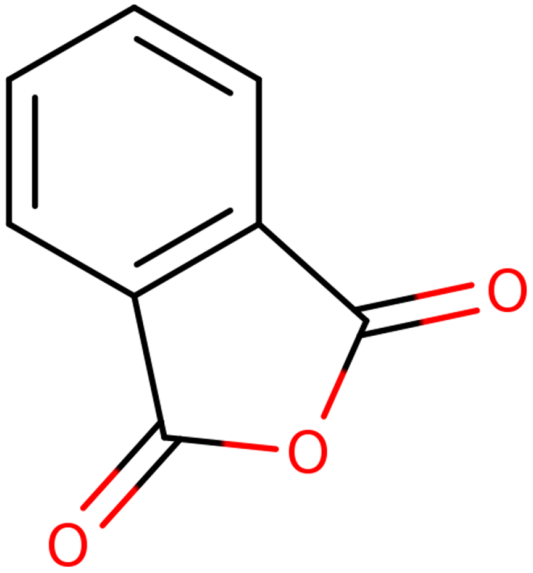
United States
Environmental Protection Agency

March 2026
Office of Chemical Safety and
Pollution Prevention

Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties for Phthalic Anhydride

Systematic Review Support Document for the Draft Risk Evaluation

CASRN: 85-44-9



March 2026

This supplemental file contains information regarding the data extraction and evaluation results for data sources that were considered for the *Draft Risk Evaluation for Phthalic Anhydride* and that underwent systematic review. EPA used the TSCA systematic review process described in the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances* (also referred to as the '2021 Draft Systematic Review Protocol'). The systematic review steps are further described in the *Draft Systematic Review Protocol for Phthalic Anhydride*. EPA conducted data extractions and data quality evaluations based on author-reported descriptions and results; additional analyses (*e.g.*, statistical analyses) potentially conducted by EPA are not contained in this supplemental file. Additionally, the overall quality determination (OQD) for each reference represents the data as a whole for each study and not for individual metric domains within a study.

Table of Contents

Phthalic acid

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Physical Form or State
HERO ID:	3981013

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Results Value	solid
Results Details	not specified

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Physical Form or State
HERO ID:	10171484

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; white needles from alcohol and benzene; Not Reported
Results Value	CRC Handbook 95th edition
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

⋆ Related References: cited from Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-460 (HERO ID HERO ID: 2828348)

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Physical Form or State
HERO ID:	10171484

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; white, lustrous needles; Not Reported
Results Value	Merck Index 2013
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: cited from O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p.1369 HERO ID: 5926376

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Physical Form or State
HERO ID:	10171484

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; colorless needles; monoclinic or rhombic prisms; Not Reported
Results Value	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Cited from International Labour Office. Encyclopedia of Occupational Health and Safety. Vols. I&II. Geneva, Switzerland: International Labour Office, 1983., p.1693 (Hero ID 63457)

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Physical Form or State
HERO ID:	10171484

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; mild odor; Not Reported
Results Value	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: cited from Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 989

Study Citation:	NCI, (1979). Bioassay of phthalic anhydride for possible carcinogenicity.
OECD Harmonized Template:	Physical Form or State
HERO ID:	63768

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Koppers Co.; white, granular solid; 98.8 % (estimated by high-pressure liquid chromatography)
Results Value	white, granular solid
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: no references cited

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.
OECD Harmonized Template:	Physical Form or State
HERO ID:	192177

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; Solid; NR Notes: NR
Results Value	White solid (flake); clear, colorless, mobile liquid (molten); characteristic, acrid odor
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Value	solid
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available and peer-reviewed database.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: NIOSH. 2010. NIOSH Pocket Guide to Chemical Hazards. Department of Health & Human Services, Centers for Disease Control & Prevention. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2010-168.

Study Citation:	O'Neil, M. J. (2013). Phthalic anhydride. 85-44-9. :1369.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926376

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Value	solid white needles
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a recognized data collection where data are peer-reviewed by experts in the field.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Rumble, J. R., (Ed.) (2018). Phthalic anhydride. :3-46.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926367

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Value	solid white needles
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a recognized data collection where data are peer-reviewed by experts in the field.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for phthalic anhydride. CAS Registry Number: 85-44-9..
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926431

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details	white

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed database that contains references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Value reported by multiple primary sources in REAXYS.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for phthalic anhydride. CAS Registry Number: 85-44-9..
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926431

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details	colorless

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed database that contains references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Value reported by multiple primary sources in REAXYS.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for phthalic anhydride. CAS Registry Number: 85-44-9..
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926431

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details	yellow

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed database that contains references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Konieczynska, Marlena D.; Dai, Chunhui; Stephenson, Corey R. J.; Organic and Biomolecular Chemistry; vol. 10; nb. 23; (2012); p. 4509 - 4511

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details	white, lustrous needles

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available and peer-reviewed database.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: O'Neil, M.J. (Ed.) 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. p. 1369.

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details	white solid (flake) or a clear colorless liquid (molten), characteristic, acrid odor.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available and peer-reviewed database.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: NIOSH. 2010. NIOSH Pocket Guide to Chemical Hazards. Department of Health & Human Services, Centers for Disease Control & Prevention. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2010-168.

Study Citation:	Das, D., Dharwadkar, S. R., Chandrasekharaiah, M. S. (1979). Vapour pressure of phthalic anhydride. Thermochimica Acta 30(1-2):371-376.
OECD Harmonized Template:	Melting Point
HERO ID:	5177115

EXTRACTION

Parameter	**Data**
Melting Point	405.5 - K
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; calculation; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	2 K
Results Details	calculated from the measured temperature dependence of the vapor pressures of solid and liquid phthalic anhydride

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Das, D., Dharwadkar, S. R., Chandrasekharaiah, M. S. (1979). Vapour pressure of phthalic anhydride. Thermochimica Acta 30(1-2):371-376.
OECD Harmonized Template:	Melting Point
HERO ID:	5177115

EXTRACTION

Parameter	**Data**
Melting Point	404.0 - K
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	0.5 K
Results Details	Observed

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used
Domain 3: Other				
	Metric 5:	Databases	High	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Melting Point
HERO ID:	3981013

EXTRACTION

Parameter	**Data**
Melting Point	130.8 - °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; none
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Results Details Methods	not reported
Standard Deviation Results	not reported
Results Details	not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for phthalic anhydride. CAS Registry Number: 85-44-9..
OECD Harmonized Template:	Melting Point
HERO ID:	5926431

EXTRACTION

Parameter	**Data**
Melting Point	123 - 134 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Measured conditions were not reported; 41 values were reported in Reaxys; 41 of these values were reported in the range of 123 to 134°C; 0 data points were outside the range.
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a secondary database with a references to the peer-reviewed original source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Data range determined from multiple primary sources in REAXYS.

Study Citation:	Monroe, K. P. (1920). Phthalic anhydride. II. The melting point of pure phthalic anhydride. the system: phthalic anhydride—phthalic acid. Journal of the Franklin Institute 189(1):103-104.
OECD Harmonized Template:	Melting Point
HERO ID:	5178041

EXTRACTION

Parameter	**Data**
Melting Point	130.84 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; Very pure chemical prepared by re-sublimation in vacuo in the presence of P2O5 Notes: NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	eutectic temperature of phthalic anhydride and phthalic acid was determined to be 129.74°C

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed primary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	NCI, (1979). Bioassay of phthalic anhydride for possible carcinogenicity.
OECD Harmonized Template:	Melting Point
HERO ID:	63768

EXTRACTION

Parameter	**Data**
Melting Point	131 - °C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Koppers Co.; solid; 98.8 % (estimated by high-pressure liquid chromatography
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	(literature: 130.8 C)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: no references cited

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.
OECD Harmonized Template:	Melting Point
HERO ID:	192177

EXTRACTION

Parameter	**Data**
Melting Point	267 - F
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Results Details Methods	NR
Standard Deviation Results	NR
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Melting Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Melting Point	403.73 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	0.2 K
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Donnelly, J.R.; Drewes, L.A.; Johnson, R.L.; Munslow, W.D.; Knapp, K.K.; Sovocool, G.W., Purity and heat of fusion data for environmental standards as determined by differential scanning calorimetry, Thermochim. Acta, 1990, 167, 2, 155, https://doi.org/10.1016/0040-6031(90)80476-F . [all data]

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Melting Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Melting Point	403 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	3.0 K
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Parks, G.S.; Todd, S.S.; Shomate, C.H., Thermal data on organic compounds. XVII. Some heat capacity, entropy and free energy data for five higher olefins, J. Am. Chem. Soc., 1936, 58, 2505.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Melting Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Melting Point	404.76 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	0.07 K
Results Details	Also report 404.75 K with standard deviation of 0.07 K under Tfus

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Marti, F.B., Methods and equipment used at the bureau of physico-chemical standards: 3 Physico-chemical properties of some solid organic compounds at normal temperatures, Bull. Soc. Chim. Belg., 1930, 39, 590.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Melting Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Melting Point	404.05 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	0.4 K
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Lombaers, R.H., Freezing of some systems containing sec-Butyl alchohol or its derivatives., Bull. Soc. Chim. Belg., 1924, 33, 232.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Melting Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Melting Point	400 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	1.5 K
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Sorum, C.H.; Durand, E.A., The Melting of Binary Eutectics, J. Am. Chem. Soc., 1952, 74, 1071.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Melting Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Melting Point	404.35 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	0.15 K
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Witschonke, C.R., Freezing point and purity data for some organic compounds, Anal. Chem., 1954, 26, 562-4.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Melting Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Melting Point	404.15 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	0.25 K
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: cited from Witschonke, C.R., Freezing point and purity data for some organic compounds, Anal. Chem., 1954, 26, 562-4.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Melting Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Melting Point	404.75 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	0.15 K
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Burriel, F., Physico-Chemical Study of Some Solid Organic Compounds at Ordinary Temperatures, and Their COrrelationo with Temperature, An. R. Soc. Esp. Fis. Quim., 1931, 29, 89.

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Melting Point
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
Melting Point	131.4 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Haynes, W.M. (Ed.) CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015. p. 3-460.

Study Citation:	O'Neil, M. J. (2013). Phthalic anhydride. 85-44-9. :1369.
OECD Harmonized Template:	Melting Point
HERO ID:	5926376

EXTRACTION

Parameter	**Data**
Melting Point	130.8 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Melting Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Melting Point	131 - 132 °C
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	Not Reported; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Source cited: MITI (Ministry of International Trade and Industry) (1992). Biodegradation andbioaccumulation data of existing chemicals based on the Chemical Substances ControlLaw (CSCL). Japan. Chemicals Inspection and Testing Institute (CITI, ed.); JapanChemicals Industry Ecology Toxicology and Information Center 3-97.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Melting Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Melting Point	123 - 134 °C
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	Not Reported; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Values were reported in the range of 123-134; 131-132 were most common; values from 36 original references.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing handbook.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Source cited: Beilstein (2002). Handbook Register Number: 118515; two entries of update dates: 2002-10-21 and 2003-10-23.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Melting Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Melting Point	130.8 - °C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	not specified
Standard Deviation Results	not specified
Results Details	not specified

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing handbook.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Source cited: Merck Index (2001). Monograph to phthalic anhydride. 13th edition, 2001 electronicrelease. Whitehouse Station, New Jersey, USA.Verschueren K (1996). Handbook of Environmental Data on Organic Chemicals (3rd ed.)Van Nostrand Reinhold, New York, p 1549.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Melting Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Melting Point	131 - °C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	not specified
Standard Deviation Results	not specified
Results Details	not specified

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Low	Secondary source citing secondary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Source cited:NIOSH (2004). http://www.cdc.gov/niosh/ipcsneng/neng0315.html (International ChemicalSafety Cards); U.S.A.Roempp (2003). Roempp Lexion Chemie (2nd electronic version), Phthalsaeureanhydrid.G. Thieme Verlag, Stuttgart.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Melting Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Melting Point	131.2 - °C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	not specified
Standard Deviation Results	not specified
Results Details	not specified

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing handbook.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Source cited:Sax NI (1979). Dangerous Properties of Industrial Materials. 5th edition, Van NostrandReinhold Company, New York, p 914.Lewis RJ (1993). Hawley´s Condensed Chemical Dictionary (12th ed.). Van NostrandReinhold, New York, p. 913.

Study Citation:	Ohm, R. F. (2000). Rubber chemicals.
OECD Harmonized Template:	Melting Point
HERO ID:	9493554

EXTRACTION

Parameter	**Data**
Melting Point	125 - 130 °C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: no references cited

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	Melting Point
HERO ID:	679796

EXTRACTION

Parameter	**Data**
Melting Point	131 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Melting Point
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Melting Point	130 - 132 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: LabNetwork

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Melting Point
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Melting Point	131 - 133 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Melting Point
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Melting Point	131 - 134 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: SynQuest

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Melting Point
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Melting Point	129 - 133 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Merck Millipore

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Melting Point
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Melting Point	130 - 134 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	Rumble, J. R. (2018). Phthalic acid. :3-46.
OECD Harmonized Template:	Melting Point
HERO ID:	7274314

EXTRACTION

Parameter	**Data**
Melting Point	131.4 °C
CASRN and Test Material	85-44-9; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Rumble, J. R., (Ed.) (2018). Phthalic anhydride. :3-46.
OECD Harmonized Template:	Melting Point
HERO ID:	5926367

EXTRACTION

Parameter	**Data**
Melting Point	131.4 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Melting Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Melting Point	131 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Merck Millipore

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Melting Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Melting Point	131 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that provides references to the original, peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: PhysProp

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Melting Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Melting Point	131 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Jean-Claude Bradley Open Melting Point Dataset

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Melting Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Melting Point	133 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: SynQuest

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Melting Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Melting Point	132 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Melting Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Melting Point	132 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Melting Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Melting Point	132 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Jean-Claude Bradley Open Melting Point Dataset

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Melting Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Melting Point	132 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Melting Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Melting Point	132 °C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Boiling Point
HERO ID:	3981013

EXTRACTION

Parameter	**Data**
Boiling Point	295 - C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Standard Deviation Results	not reported
Results Details	@ 760 mm Hg

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for phthalic anhydride. CAS Registry Number: 85-44-9..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926431

EXTRACTION

Parameter	**Data**
Boiling Point	284.5 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	@ 760 torr; 8 values were reported in Reaxys; 1 value was reported as 284.5 C at 760 torr; 7 values were outside this range or measured at unreported or non-standard pressures.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a secondary database with a references to the peer-reviewed original source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

⋆ Related References: Data range determined from multiple primary sources in REAXYS.

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Boiling Point
HERO ID:	10171484

EXTRACTION

Parameter	**Data**
Boiling Point	791.0 - K
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	Not Reported
Results Details	reported as critical temperature (est,)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Supplement 1. Design Institute for PhysicalProperty Data, American Institute of Chemical Engineers, Hemisphere Pub. Corp., New York, NY (1991)

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.
OECD Harmonized Template:	Boiling Point
HERO ID:	192177

EXTRACTION

Parameter	**Data**
Boiling Point	563 - F
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; None
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Standard Deviation Results	NR
Results Details	at 1 atmosphere

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Boiling Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Boiling Point	557.83 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	0.3 K
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Burriel, F., Physico-Chemical Study of Some Solid Organic Compounds at Ordinary Temperatures, and Their COrrelationo with Temperature, An.R. Soc. Esp. Fis. Quim., 1931, 29, 89.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Boiling Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Boiling Point	557.2 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Aldrich Chemical Company Inc., Catalog Handbook of Fine Chemicals, Aldrich Chemical Company, Inc., Milwaukee WI, 1990, 1

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Boiling Point
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Boiling Point	558.25 - K
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	0.3 K
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Burriel, F., Physico-Chemical Study of Some Solid Organic Compounds at Ordinary Temperatures, and Their COrrelationo with Temperature, An.R. Soc. Esp. Fis. Quim., 1931, 29, 89.

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
Boiling Point	285.3 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Haynes, W.M. (Ed.) CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015. p. 3-460.

Study Citation:	O'Neil, M. J. (2013). Phthalic anhydride. 85-44-9. :1369.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926376

EXTRACTION

Parameter	**Data**
Boiling Point	295 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	sublimes

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Boiling Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Boiling Point	284.5 - C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	not specified
Results Details	Pressure assumed to be 1013 hPa

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Source cited: MITI (Ministry of International Trade and Industry) (1992). Biodegradation andbioaccumulation data of existing chemicals based on the Chemical Substances ControlLaw (CSCL). Japan. Chemicals Inspection and Testing Institute (CITI, ed.); JapanChemicals Industry Ecology Toxicology and Information Center 3-97.Verschueren K (1996). Handbook of Environmental Data on Organic Chemicals (3rd ed.)Van Nostrand Reinhold, New York, p 1549.Auergesellschaft GmbH (1988). Auer Technikum. Berlin, 12. ed., 518-520.Towle PH, Baldwin RH, Meyer DH (1968). Phthalic acids. In: Kirk-Othmer, Encycl. Chem.Tech. 2nd ed. 15, 444-456.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Boiling Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Boiling Point	295 - C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	not specified
Results Details	at 1013 hPa

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. Multiple sources cited same value.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Source cited: Merck Index (2001). Monograph to phthalic anhydride. 13th edition, 2001 electronicrelease. Whitehouse Station, New Jersey, USA.Lorz PM, Towae FK, Bhargava N (2002). Ullmann Encyclopedia of Industrial Chemistry.Phthalic Acid and Derivatives (electronic edition). Wiley-VCH Verlag, Weinheim.Merck Index (2001). Monograph to phthalic anhydride. 13th edition, 2001 electronicrelease. Whitehouse Station, New Jersey, USA.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Boiling Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Boiling Point	285 - C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	not specified
Results Details	not specified

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing handbook.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Source cited: Roempp (2003). Roempp Lexion Chemie (2nd electronic version), Phthalsaeureanhydrid.G. Thieme Verlag, Stuttgart.Chemicals Industry Ecology Toxicology and Information Center 3-97.Lewis RJ (1993). Hawley´s Condensed Chemical Dictionary (12th ed.). Van NostrandReinhold, New York, p. 913.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Boiling Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Boiling Point	295 - C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	not specified
Results Details	at 1013 hPa

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing handbook.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Source cited: Sax NI (1979). Dangerous Properties of Industrial Materials. 5th edition, Van NostrandReinhold Company, New York, p 914.Reinhold, New York, p. 913.

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	Boiling Point
HERO ID:	679796

EXTRACTION

Parameter	**Data**
Boiling Point	284.5 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Standard Deviation Results	NR
Results Details	Sublimates

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Boiling Point	284 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: LabNetwork

Study Citation:	Rumble, J. R. (2018). Flammability of chemical substances. :16-16 - 16-32.
OECD Harmonized Template:	Boiling Point
HERO ID:	6655446

EXTRACTION

Parameter	**Data**
Boiling Point	285.3
CASRN and Test Material	Not Reported; Phthalic anhydride
Confidentiality, Type, and Guideline	none; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Standard Deviation Results	Not reported
Results Details	Not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a known data-collection, prepared by experts in the field.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Rumble, J. R. (2018). Phthalic acid. :3-46.
OECD Harmonized Template:	Boiling Point
HERO ID:	7274314

EXTRACTION

Parameter	**Data**
Boiling Point	285.5 C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	No; experimental; NR
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Standard Deviation Results	NR
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Rumble, J. R., (Ed.) (2018). Phthalic anhydride. :3-46.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926367

EXTRACTION

Parameter	**Data**
Boiling Point	285.3 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Boiling Point	295 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that provides references to the original, peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: PhysProp

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Boiling Point	295 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that references a peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: NIOSH

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Boiling Point	295 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Boiling Point	295 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Boiling Point	284 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: SynQuest

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Density
HERO ID:	3981013

EXTRACTION

Parameter	**Data**
Density	1.527 -
CASRN and Test Material	85-44-9; Phthalic acid
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Density Type	specific gravity (density of a substance divided by the density of water)
System	not specified
Temperature	4°C
Standard Deviation Results	not reported
Results Details	not reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Density
HERO ID:	10171484

EXTRACTION

Parameter	**Data**
Density	6.6 -
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	vapor density
System	Not Reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from CDC; International Chemical Safety Cards (ICSC) 2012. Atlanta, GA: Centers for Disease Prevention & Control. National Institute for OccupationalSafety & Health (NIOSH). Ed Info Div. Available from, as of Jan 28, 2015: http://www.cdc.gov/niosh/ipcs/icstart.html

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.
OECD Harmonized Template:	Density
HERO ID:	192177

EXTRACTION

Parameter	**Data**
Density	1.20 (molten) - 1.53 (flake) Not reported
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; NR
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Density Type	Specific gravity
System	Not reported
Temperature	Not Reported
Standard Deviation Results	NR
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information

Overall Quality Determination — Medium

Study Citation:	NIOSH, (1978). Occupational health guideline for phthalic anhydride.
OECD Harmonized Template:	Density
HERO ID:	8408508

EXTRACTION

Parameter	**Data**
Density	5.1 - not reported
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	Vapor Density
System	Not Reported
Temperature	at the boiling point of phthalic anhydride
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: no references cited

Study Citation:	NIOSH, (1978). Occupational health guideline for phthalic anhydride.
OECD Harmonized Template:	Density
HERO ID:	8408508

EXTRACTION

Parameter	Data
Density	1.5 - not reported
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	Specific Gravity
System	Not Reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: no references cited

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Density
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Density	1.527 - g/cm3
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	relative density
System	not reported
Temperature	20C
Standard Deviation Results	not specified
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing handbook.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Source cited: Beilstein (2002). Handbook Register Number: 118515; two entries of update dates: 2002-10-21 and 2003-10-23.Lorz PM, Towae FK, Bhargava N (2002). Ullmann Encyclopedia of Industrial Chemistry.Phthalic Acid and Derivatives (electronic edition). Wiley-VCH Verlag, Weinheim.Roempp (2003). Roempp Lexion Chemie (2nd electronic version), Phthalsaeureanhydrid.G. Thieme Verlag, Stuttgart.Merck Index (2001). Monograph to phthalic anhydride. 13th edition, 2001 electronicrelease. Whitehouse Station, New Jersey, USA.NIOSH (2004). http://www.cdc.gov/niosh/ipcsneng/neng0315.html (International ChemicalSafety Cards); U.S.A.Verschueren K (1996). Handbook of Environmental Data on Organic Chemicals (3rd ed.)Van Nostrand Reinhold, New York, p 1549.Sax NI (1979). Dangerous Properties of Industrial Materials. 5th edition, Van NostrandReinhold Company, New York, p 914.Lewis RJ (1993). Hawley´s Condensed Chemical Dictionary (12th ed.). Van NostrandReinhold, New York, p. 913.Auergesellschaft GmbH (1988). Auer Technikum. Berlin, 12. ed., 518-520.Towle PH, Baldwin RH, Meyer DH (1968). Phthalic acids. In: Kirk-Othmer, Encycl. Chem.Tech. 2nd ed. 15, 444-456.

Study Citation:	Ohm, R. F. (2000). Rubber chemicals.
OECD Harmonized Template:	Density
HERO ID:	9493554

EXTRACTION

Parameter	**Data**
Density	1.48 - Mg/m3
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	Density
System	Not Reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: no references cited

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	Density
HERO ID:	679796

EXTRACTION

Parameter	**Data**
Density	1.527
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Density Type	density reported as specific gravity
System	NR
Temperature	4 deg C
Standard Deviation Results	NR
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Rumble, J. R. (2018). Phthalic acid. :3-46.
OECD Harmonized Template:	Density
HERO ID:	7274314

EXTRACTION

Parameter	**Data**
Density	1.527 - g/cm3
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	none; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	density
System	not specified
Temperature	4
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for phthalic anhydride. CAS Registry Number: 85-44-9..
OECD Harmonized Template:	Density
HERO ID:	5926431

EXTRACTION

Parameter	**Data**
Density	1.527 g/cm3
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	20°C
Standard Deviation Results	Not Reported
Results Details	20°C; 7 values were reported in Reaxys; 1 value was reported as 1.527 at 20 C; 6 values were measured at non-standard or unreported temperatures.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a secondary database with a references to the peer-reviewed original source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Gevorkyan, A. A.; Amitin, A. V.; Gorelik, A. G. Journal of applied chemistry of the USSR, 1983, vol. 56, # 12, p. 2563 - 2565

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Density
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
Density	1.20 - 1.53 g/cm3
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	1.20 molten, 1.53 flake

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: NIOSH. 2010. NIOSH Pocket Guide to Chemical Hazards. Department of Health & Human Services, Centers for Disease Control & Prevention. National Institute for Occupational Safety & Health. DHHS (NIOSH) Publication No. 2010-168.

Study Citation:	O'Neil, M. J. (2013). Phthalic anhydride. 85-44-9. :1369.
OECD Harmonized Template:	Density
HERO ID:	5926376

EXTRACTION

Parameter	**Data**
Density	1.53 g/cm3
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Density
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Density	1.53 g/cm3
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: SynQuest

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Density
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Density	1.53 g/cm3
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	Rumble, J. R., (Ed.) (2018). Phthalic anhydride. :3-46.
OECD Harmonized Template:	Density
HERO ID:	5926367

EXTRACTION

Parameter	**Data**
Density	1.527 g/cm3
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	4°C
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic anhydride.
OECD Harmonized Template:	Density
HERO ID:	6592047

EXTRACTION

Parameter	**Data**
Density	5.1
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	Relative to air

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: NTP, 1992. CAMEO Chemicals.

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic anhydride.
OECD Harmonized Template:	Density
HERO ID:	6592047

EXTRACTION

Parameter	**Data**
Density	5.1
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	air = 1

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: ILO International Chemical Safety Cards (ICSC)

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic anhydride.
OECD Harmonized Template:	Density
HERO ID:	6592047

EXTRACTION

Parameter	**Data**
Density	5.1
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Occupational Safety and Health Administration (OSHA)

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Density
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
Density	6.6
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	air = 1

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: CDC. 2012. International Chemical Safety Cards (ICSC). Atlanta, GA: Centers for Disease Prevention & Control. National Institute for Occupational Safety & Health (NIOSH). Ed Info Div.

Study Citation:	Antipin, A. V., Vakurova, E. A., Katunin, V. K., AFANASEV.NS (1972). Vapor-pressure of solid phthalic anhydride. Russian Journal of Physical Chemistry A, Focus on Chemistry 46(4):619-619.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5180233

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; purification via repeated crystallization at 131.2C
Temperature	40-110°C
System	Saturation method (inert gas jet method) for the determination of an Equation for vapor pressure of solid phthalic anhydride over the temperature range of 30-130C
Standard Deviation Results	Not applicable
Results Details	log p (pressure) = (12.1663±0.2)-[(4592.957±74.535)/T]

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

Study Citation:	Das, D., Dharwadkar, S. R., Chandrasekharaiah, M. S. (1979). Vapour pressure of phthalic anhydride. Thermochimica Acta 30(1-2):371-376.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5177115

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; liquid; Reagent Grade. Further purified by resubliming twice.
Temperature	Not Reported
System	Carrier gas entrainment method
Standard Deviation Results	Not Reported
Results Details	Enthalpy of Vaporization at 422 K : 63.9 +/- 2.5 kJ/molcalculated using the second law method.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Data measured for a structural analogue of the subject chemical substance are consistent with what is expected for the subject chemical substance structural properties, features or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Das, D., Dharwadkar, S. R., Chandrasekharaiah, M. S. (1979). Vapour pressure of phthalic anhydride. Thermochimica Acta 30(1-2):371-376.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5177115

EXTRACTION

Parameter	**Data**
Vapor Pressure	2.2 - Pa
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; solid; Reagent Grade. Further purified by resubliming twice.
Temperature	333 +/- 0.5 K
System	Carrier gas entrainment method
Standard Deviation Results	Not Reported
Results Details	vapor pressure reported as partial pressure of phthalic anhydride. Other data points listed below:2.3 Pa at 333.6 K3.9 Pa at 341.0 K10.5 Pa at 351.6 K9.8 Pa at 353.7 K21.4 Pa at 361.2 K21.2 Pa at 363.6 K60.8 Pa at 375.0 K66.9 Pa at 375.4 K94.1 Pa at 382.0 K260.1 Pa at 395.7 K259.9 Pa at 395.9 K411.9 Pa at 403.8 K

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Data measured for a structural analogue of the subject chemical substance are consistent with what is expected for the subject chemical substance structural properties, features or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Das, D., Dharwadkar, S. R., Chandrasekharaiah, M. S. (1979). Vapour pressure of phthalic anhydride. Thermochimica Acta 30(1-2):371-376.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5177115

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	tensimetric technique
Standard Deviation Results	Not Reported
Results Details	Enthalpy of vapor pressure: 65.3 +/- 0.8 kJ/molNotes that the available experimental details to obtain value are insufficient.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Data measured for a structural analogue of the subject chemical substance are consistent with what is expected for the subject chemical substance structural properties, features or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Cited from D. A. Creeks and F. M. Feetham, J- Chem. Sac., (1946) 899.

Study Citation:	Das, D., Dharwadkar, S. R., Chandrasekharaiah, M. S. (1979). Vapour pressure of phthalic anhydride. Thermochimica Acta 30(1-2):371-376.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5177115

EXTRACTION

Parameter	**Data**
Vapor Pressure	589.5 - Pa
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; liquid; Reagent Grade. Further purified by resubliming twice.
Temperature	441.7 +/- 0.5 K
System	Carrier gas entrainment method
Standard Deviation Results	Not Reported
Results Details	vapor pressure reported as partial pressure of phthalic anhydride. Other data points listed below:608.1 Pa at 411.7 K887.8 Pa at 419.5 K823.3 Pa at 420.1 K1552.0 Pa at431.9 K1406.7 Pa at 432.9 K20242.8 Pa at 440.2 K1993.8 Pa at 440.5 K

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Data measured for a structural analogue of the subject chemical substance are consistent with what is expected for the subject chemical substance structural properties, features or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	3981013

EXTRACTION

Parameter	**Data**
Vapor Pressure	7.5x10-3 - mm Hg
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Temperature	48.2°C
System	not reported
Standard Deviation Results	not reported
Results Details	not reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	10171484

EXTRACTION

Parameter	**Data**
Vapor Pressure	4.72 x 10+6 - Pa
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	reported as critical pressure

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Cited from Daubert TE, Danner RP; Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Supplement 1. Design Institute for PhysicalProperty Data, American Institute of Chemical Engineers, Hemisphere Pub. Corp., New York, NY (1991)

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	192177

EXTRACTION

Parameter	**Data**
Vapor Pressure	0.0015 - mm Hg
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Temperature	NR
System	NR
Standard Deviation Results	NR
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Enthalpy of Vaporization: 54.1 kJ/mol at 521 K

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Monroe, K.P., Phthalic Anhydride. IV—The Vapor Pressure of Phthalic Anhydride, J. Ind. Eng. Chem., 1920, 12, 10, 969-971,https://doi.org/10.1021/ie50130a013

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Enthalpy of Vaporization: 52.1 kJ/mol at 422 KCalculated from the vapor pressure data reported by the method of least squares

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Stephenson, Richard M.; Malanowski, Stanislaw, Handbook of the Thermodynamics of Organic Compounds, 1987,https://doi.org/10.1007/978-94-009-3173-2 .

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Phthalic anhydride (85-44-9). Standard Reference Database No. 69.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	10225179

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Enthalpy of Vaporization: 63.9 +/- 2.5 kJ/mol at 422 KGas saturation, transpiration

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from Das, D.; Dharwadkar, S.R.; Chandrasekharaiah, M.S., Vapour pressure of phthalic anhydride, Thermochimica Acta, 1979, 30, 1-2, 371-376,https://doi.org/10.1016/0040-6031(79)85076-5

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
Vapor Pressure	5.17E-4 mm Hg
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	25°C
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Jones, A.H. 1960. J Chem Eng Data. 5: 196-200.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Vapor Pressure	0.0006 hPa
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified: Menzies's method (30°-60°C), mercury manometer (90°-145°C)
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	26.6C
System	not specified
Standard Deviation Results	not specified
Results Details	Values ranged from 0.000041 to 13.2 hPa at a temperatures of 1.5 to 143.2 °C.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Source cited: HERO ID 5348321 Crooks DA and Feetham FM (1946). The vapour pressure of phthalic anhydride. J. Chem. Soc.,899-901.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Vapor Pressure	0.032 hPa
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25C
System	not specified
Standard Deviation Results	not specified
Results Details	methodological deficiencies noted

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing handbook.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Source cited: Yaws CL (1994). Handbook of Vapor Pressure. Volume 3 - C8 to C28 Compounds. GulfPublishing Company, Houston, Texas.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5160034

EXTRACTION

Parameter	Data
Vapor Pressure	8 (6) - 1013 (760) hPa (mm Hg)
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	132-284.5C
System	not specified
Standard Deviation Results	not specified
Results Details	not specified

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Low	Secondary source citing Secondary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Source cited: Towle PH, Baldwin RH, Meyer DH (1968). Phthalic acids. In: Kirk-Othmer, Encycl. Chem.Tech. 2nd ed. 15, 444-456. (HERO ID 5348322 not in distiller at time of extraction)

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Vapor Pressure	0.00027 hPa
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	20C
System	not specified
Standard Deviation Results	not specified
Results Details	other values reported 0.0013 hPa at 30°C and 0.02 hPa at 50°C

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other			
Metric 5:	Databases	Medium	Secondary source citing handbook.
Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Source cited: Auergesellschaft GmbH (1988). Auer Technikum. Berlin, 12. ed., 518-520.Verschueren K (1996). Handbook of Environmental Data on Organic Chemicals (3rd ed.)Van Nostrand Reinhold, New York, p 1549.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Vapor Pressure	ca. 173.6 - 1009.9 hPa
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	212 to 284.6C
System	not specified
Standard Deviation Results	not specified
Results Details	other values are:ca. 1.33 - 1010.8 hPa at 96.5 - 284.5 °Cca. 0.0004 - 13.1 hPa at 1.5 - 143.2 °C

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Low	Secondary source citing secondary handbook source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Source cited: Beilstein (2002). Handbook Register Number: 118515; two entries of update dates: 2002-10-21 and 2003-10-23.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Vapor Pressure	< 0.003 hPa
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	20C
System	not specified
Standard Deviation Results	not specified
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Low	Secondary source citing secondary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Source cited: NIOSH (2004). http://www.cdc.gov/niosh/ipcsneng/neng0315.html (International ChemicalSafety Cards); U.S.A.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Vapor Pressure	0.000689 hPa
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; Mcleod gage method
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25C
System	not specified
Standard Deviation Results	not specified
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Source cited: Jones AH (1960). Sublimation pressure data for organic compounds. J. Chem. Eng. Data,5: 196-200. (HERO ID 5348318 not in distiller at time of extraction)

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	679796

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; heat of vaporization
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Temperature	131 deg C
System	Not reported
Standard Deviation Results	NR
Results Details	65.3 kJ/mol

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Vapor Pressure	0.0015 mm Hg
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that references a peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: NIOSH

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Vapor Pressure	5.17E-4 mm Hg
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that provides references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: PhysProp. Jones, AH 1960

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for phthalic anhydride. CAS Registry Number: 85-44-9..
OECD Harmonized Template:	logKow
HERO ID:	5926431

EXTRACTION

Parameter	**Data**
log k_{ow}	1.43
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	Measured conditions were not reported.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a secondary database with a references to the peer-reviewed original source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Magenau, Andrew J. D.; Richards, Jeffrey A.; Pasquinelli, Melissa A.; Savin, Daniel A.; Mathers, Robert T.; Macromolecules; vol. 48; nb. 19; (2015); p. 7230 - 7236

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	logKow
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
log k_{ow}	1.6
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available and peer-reviewed database that references a review document.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: OECD. 2005. SIDS Initial Assessment Report for SIAM 20, Phthalic Anhydride (85-44-9).

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	logKow
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
log k_{ow}	0.73 -
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; calculation; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	not specified
System	not specified
pH	1
Results Details Method	not specified
Standard Deviation Results	not specified
Results Details	Phthalic acid is the major organic degradation product of phthalic anhydridehydrolysis

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	Medium	Data are measured for hydrolysis product of the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Source cited: HERO ID 5349292 (not in distiller at time of extrcation)

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	logKow
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
log k_{ow}	1.6 -
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	not specified
System	not specified
pH	not specified
Results Details Method	not specified
Standard Deviation Results	not specified
Results Details	Rapid hydrolysis to phthalic acid

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Low	Secondary source citing secondary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Source cited: NIOSH (2003). International Chemical Safety Card 0315. Phthalic anhydride. http://www.cdc. gov/niosh/ipcsneng/neng0315.html.

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	logKow
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
log k_{ow}	1.6
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that references peer-reviewed original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: PhysProp. Hansch, C et al. 1995

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Water Solubility
HERO ID:	10171484

EXTRACTION

Parameter	**Data**
Water Solubility	16400 - mg/L
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	including rapid hydrolysis to phthalic acid

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

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Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Water Solubility
HERO ID:	10171484

		EVALUATION	
Domain	Metric	Rating	Comments
Overall Quality Determination		**High**	

* Related References: cited from OECD; SIDS Initial Assessment Report For SIAM 20, Phthalic Anhydride (85-44-9), April 2005. Available from, as of Jan 27, 2015:http://www.chem.unep.ch/irptc/sids/OECDSIDS/85449.pdf (HERO ID 5160034)

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Water Solubility
HERO ID:	10171484

EXTRACTION

Parameter	Data
Water Solubility	6200 - 6400 mg/L
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	20-25 C
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	(ECHA)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from ECHA; Search for Chemicals. Phthalic Anhydride (85-44-9) Registered Substances Dossier. European Chemical Agency. Available from, as of Jan 28,2015: http://echa.europa.eu/

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Water Solubility
HERO ID:	10171484

EXTRACTION

Parameter	Data
Water Solubility	162 - parts water
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	more in hot watersoluble in 162 parts water

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: cited from O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p.1369 (HERO ID: 5926376)

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Water Solubility
HERO ID:	10171484

EXTRACTION

Parameter	Data
Water Solubility	6200 - mg/L
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	26
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	also reports 5,964 mg/L at room temperature

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Yalkowsky, S.H., He, Yan, Jain, P. Handbook of Aqueous Solubility Data Second Edition. CRC Press, Boca Raton, FL 2010, p. 448 (HERO ID: 2990992)

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.
OECD Harmonized Template:	Water Solubility
HERO ID:	192177

EXTRACTION

Parameter	**Data**
Water Solubility	0.6 - g/100 ml
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Temperature	68
System	NR
pH	NR
Results Details Method	NR
Standard Deviation Results	NR
Results Details	Solubility in water at 68°F reported as % by weight (g/100 ml)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	NIOSH, (1978). Occupational health guideline for phthalic anhydride.
OECD Harmonized Template:	Water Solubility
HERO ID:	8408508

EXTRACTION

Parameter	**Data**
Water Solubility	0.62 - g/100 ml
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	20 C (68 F)
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	reacts slowly

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

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Study Citation:	NIOSH, (1978). Occupational health guideline for phthalic anhydride.
OECD Harmonized Template:	Water Solubility
HERO ID:	8408508

EVALUATION

Domain	Metric	Rating	Comments
Overall Quality Determination		**High**	

* Related References: no references cited

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Water Solubility
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
Water Solubility	6000 mg/L
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	25°C
System	Not Reported
pH	Not reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that provides references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Park, M.N., Sheehan, R.J. 2000. Phthalic Acids and Other Benzenepolycarboxylic Acids. Kirk-Othmer Encyclopedia of Chemical Technology. New York, NY: John Wiley & Sons.

Study Citation:	O'Neil, M. J. (2013). Phthalic anhydride. 85-44-9. :1369.
OECD Harmonized Template:	Water Solubility
HERO ID:	5926376

EXTRACTION

Parameter	**Data**
Water Solubility	6170 mg/L
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
System	Not Reported
pH	Not reported
Results Details Method	Originally reported as soluble in 162 parts water
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: O'Neil, M.J. (Ed.). 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. p. 1369.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Water Solubility
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Water Solubility	16400 - mg/L
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	20
System	not reported
pH	not reported
Results Details Method	not reported
Standard Deviation Results	not reported
Results Details	Rapid hydrolysis to phthalic acid

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Low	Source citing another secondary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Source cited: HERO 679771 Lorz PM, Towae FK, and Bhargava N (2002). Ullmann Encyclopedia of Industrial Chemistry. Phthalic Acid and Derivatives (electronic edition). Wiley-VCH Verlag, Weinheim.

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	Water Solubility
HERO ID:	679796

EXTRACTION

Parameter	**Data**
Water Solubility	6000 mg/L
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 0.6 g/100g water at 25 deg C and reported as 16.5 g/100 g water at 100 deg C and 147 g/100g at 150 deg C

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Water Solubility
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Water Solubility	6000 mg/L
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
System	Not Reported
pH	Not reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that references a peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: NIOSH

Study Citation:	Rumble, J. R. (2018). Aqueous solubility and Henry's law constants of organic compounds. :5-148 - 5-177.
OECD Harmonized Template:	Water Solubility
HERO ID:	5932745

EXTRACTION

Parameter	**Data**
Water Solubility	6200 mg/L
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	27°C
System	Not Reported
pH	Not reported
Results Details Method	Originally reported as 6.2 g/kg H20, converted using CRC handbook's reported water density at 27 C.
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Rumble, J. R. (2018). Phthalic acid. :3-46.
OECD Harmonized Template:	Water Solubility
HERO ID:	7274314

EXTRACTION

Parameter	**Data**
Water Solubility	Not Reported
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	sl in water, ether; s in EtOH, ace, bz

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Low

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Phthalic anhydride. 85-44-9..
OECD Harmonized Template:	Water Solubility
HERO ID:	5926156

EXTRACTION

Parameter	**Data**
Water Solubility	6200 mg/L
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	Not Reported
System	Not Reported
pH	Not reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that provides references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: PhysProp. Towle, PH et al. 1968

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.
OECD Harmonized Template:	Flash Point
HERO ID:	192177

EXTRACTION

Parameter	**Data**
Flash Point	305 - F
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; closed cup
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
System	closed cup
Standard Deviation Results	NR
Results Details	NR

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	NIOSH, (1978). Occupational health guideline for phthalic anhydride.
OECD Harmonized Template:	Flash Point
HERO ID:	8408508

EXTRACTION

Parameter	**Data**
Flash Point	151 - C
CASRN and Test Material	85-44-9; Not Reported
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	closed cup
Standard Deviation Results	Not Reported
Results Details	also reports 304 F

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: no references cited

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Flash Point
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
Flash Point	305 F
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Closed cup
Standard Deviation Results	Not reported
Results Details	152°C

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: National Fire Protection Association; Fire Protection Guide to Hazardous Materials. 14TH Edition, Quincy, MA 2010, p. 325-99

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Flash Point
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
Flash Point	329 F
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Open cup
Standard Deviation Results	Not reported
Results Details	305°F closed cup

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: U.S. Coast Guard, Department of Transportation. CHRIS - Hazardous Chemical Data. Volume II. Washington, D.C.: U.S. Government Printing Office, 1984-5.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Flash Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Flash Point	151.7 - C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	closed cup
Standard Deviation Results	not specified
Results Details	not specified

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing handbook value.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Source cited: Sax NI (1979). Dangerous Properties of Industrial Materials. 5th edition, Van NostrandReinhold Company, New York, p 914.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Flash Point
HERO ID:	5160034

EXTRACTION

Parameter	Data
Flash Point	152 - C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	closed cup
Standard Deviation Results	not specified
Results Details	not specified

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing secondary source and handbook value.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Source cited: NIOSH (2003). International Chemical Safety Card 0315. Phthalic anhydride. http://www.cdc. gov/niosh/ipcsneng/neng0315.html.Merck KGaA (2002). http://chemdat.merck.de (Technical Data Sheet 800592,Phthalsaeureanhydrid zur Synthese); D-64271 Darmstadt (Germany).

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Flash Point
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Flash Point	151.6 - C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	closed cup
Standard Deviation Results	not specified
Results Details	not specified

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing handbook value.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Source cited: Lewis RJ (1993). Hawley´s Condensed Chemical Dictionary (12th ed.). Van NostrandReinhold, New York, p. 913.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Flash Point
HERO ID:	5160034

EXTRACTION

Parameter	Data
Flash Point	151 - C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	closed cup
Standard Deviation Results	not specified
Results Details	not specified

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Low	Secondary source citing secondary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Source cited: Towle PH, Baldwin RH, Meyer DH (1968). Phthalic acids. In: Kirk-Othmer, Encycl. Chem. Tech. 2nd ed. 15, 444-456. (HERO ID 5348322 not in distiller at time of extraction)

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	Flash Point
HERO ID:	679796

EXTRACTION

Parameter	**Data**
Flash Point	151 - 165 deg C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; closed cup and open cup
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
System	165 deg C open cup and 151 deg C closed cup
Standard Deviation Results	NR
Results Details	NR

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Flash Point
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Flash Point	152 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Alfa Aesar

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Flash Point
HERO ID:	5926272

EXTRACTION

Parameter	Data
Flash Point	152 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that provides references to the original, peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Sigma-Aldrich

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Flash Point
HERO ID:	5926272

EXTRACTION

Parameter	Data
Flash Point	152 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not Reported
Standard Deviation Results	Not reported
Results Details	152 (305 F)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that provides references to the original, peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: NIOSH

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Flash Point
HERO ID:	5926272

EXTRACTION

Parameter	**Data**
Flash Point	152 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: SynQuest

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Flash Point
HERO ID:	5926272

EXTRACTION

Parameter	Data
Flash Point	305.6 F
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not Reported
Standard Deviation Results	Not reported
Results Details	152°C (305.6°F)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	RSC, (2019). ChemSpider: Phthalic anhydride.
OECD Harmonized Template:	Flash Point
HERO ID:	5926272

EXTRACTION

Parameter	Data
Flash Point	152 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: LabNetwork

Study Citation:	Rumble, J. R. (2018). Flammability of chemical substances. :16-16 - 16-32.
OECD Harmonized Template:	Flash Point
HERO ID:	6655446

EXTRACTION

Parameter	**Data**
Flash Point	152 C
CASRN and Test Material	Not Reported; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a known data-collection, prepared by experts in the field.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic anhydride.
OECD Harmonized Template:	Autoflammability
HERO ID:	6592047

EXTRACTION

Parameter	**Data**
Auto-flammability	1058 F
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not reported
Standard Deviation Results	Not Reported
Results Details	1058°F
Results Value	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: CAMEO Chemicals

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic anhydride.
OECD Harmonized Template:	Autoflammability
HERO ID:	6592047

EXTRACTION

Parameter	Data
Auto-flammability	570 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not reported
Standard Deviation Results	Not Reported
Results Details	570°C
Results Value	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: ILO International Chemical Safety Cards (ICSC)

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Autoflammability
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
Auto-flammability	570 C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not reported
Standard Deviation Results	Not Reported
Results Details	570°C; 1058°F
Results Value	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Hazardous Substances Data Bank (HSDB)

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Autoflammability
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Auto-flammability	580 - C
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	not specified
Standard Deviation Results	not specified
Results Details	not specified
Results Value	not specified

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Low	Source citing secondary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Source cited: HERO 679771 Lorz PM, Towae FK, and Bhargava N (2002). Ullmann Encyclopedia of Industrial Chemistry. Phthalic Acid and Derivatives (electronic edition). Wiley-VCH Verlag, Weinheim.

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	Autoflammability
HERO ID:	679796

EXTRACTION

Parameter	**Data**
Auto-flammability	584 deg C
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
System	Not reported
Standard Deviation Results	NR
Results Details	NR
Results Value	NR

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Rumble, J. R. (2018). Flammability of chemical substances. :16-16 - 16-32.
OECD Harmonized Template:	Autoflammability
HERO ID:	6655446

EXTRACTION

Parameter	**Data**
Auto-flammability	570 C
CASRN and Test Material	Not Reported; Phthalic anhydride
Confidentiality, Type, and Guideline	None; not specified; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Not reported
Standard Deviation Results	Not reported
Results Details	Not reported
Results Value	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a known data-collection, prepared by experts in the field.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Viscosity
HERO ID:	10171484

EXTRACTION

Parameter	**Data**
Viscosity	1.125 -
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	155 C
Test Conditions	Not Reported
Standard Deviation Results	Not Reported
Results Details	1.125 mPa.s (ECHA)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cited from ECHA; Search for Chemicals. Phthalic Anhydride (85-44-9) Registered Substances Dossier. European Chemical Agency. Available from, as of Jan 28,2015: http://echa.europa.eu/

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Phthalic anhydride, 85-44-9.
OECD Harmonized Template:	Viscosity
HERO ID:	5926125

EXTRACTION

Parameter	**Data**
Viscosity	1.19
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	132°C
Test Conditions	Not Reported
Standard Deviation Results	Not Reported
Results Details	1.19 mPa.S

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: ECHA. 2015. Search for Chemicals. Phthalic Anhydride (85-44-9) Registered Substances Dossier. European Chemical Agency.

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Viscosity
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Viscosity	5.5 (220C); 6.4 (197C) - 11.9 (132C)
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; molten; Not Reported
Temperature	155C
Test Conditions	dynamic
Standard Deviation Results	Not Reported
Results Details	0.875 mPa s at 180°C

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Secondary source citing handbook.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Source cited: Towle PH, Baldwin RH, Meyer DH (1968). Phthalic acids. In: Kirk-Othmer, Encycl. Chem. Tech. 2nd ed. 15, 444-456. (HERO ID 5348322 not in distiller at time of extraction)

Study Citation:	OECD, (2005). SIDS Initial Assessment Report: Phthalic anhydride. :213.
OECD Harmonized Template:	Viscosity
HERO ID:	5160034

EXTRACTION

Parameter	**Data**
Viscosity	1.125 -
CASRN and Test Material	85-44-9; Phthalic anhydride
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	155C
Test Conditions	dynamic
Standard Deviation Results	Not Reported
Results Details	0.875 mPa s at 180°C

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other			
Metric 5:	Databases	Medium	Secondary source citing handbook.
Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Source cited: Beilstein (2002). Handbook Register Number: 118515; two entries of update dates: 2002-10-21 and 2003-10-23.

Study Citation:	Canada,, Health (2019). Screening assessment carboxylic acid anhydrides group.
OECD Harmonized Template:	Henry's Law
HERO ID:	8404079

EXTRACTION

Parameter	**Data**
Henry's Law	-7.79 - log (Pa·m3/mol)
CASRN and Test Material	Not Reported; Not Reported
Confidentiality, Type, and Guideline	none; estimated; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25C
pH	not specified
System	not specified
Standard Deviation Results	Not Reported
Results Details	Not Reported
Results Details Methods	estimated, ChemIDplus

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Low	Secondary source citing secondary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Source cited: (not available at time of extration)[ChemIDplus] 1993- a. ChemIDplus [database]. Search results for CAS RN 85-44-9 . Bethesda (MD): USNational Library of Medicine. [updated 2016 July 20; accessed 2016 August 01].

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Henry's Law
HERO ID:	10171484

EXTRACTION

Parameter	**Data**
Henry's Law	1.7 x 10-8 - atm-cu m/mol
CASRN and Test Material	85-44-9; phthalic anhydride
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
pH	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported
Results Details Methods	Estimation

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

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Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6811 Phthalic anhydride.
OECD Harmonized Template:	Henry's Law
HERO ID:	10171484

		EVALUATION	
Domain	Metric	Rating	Comments
Overall Quality Determination		**Medium**	

* Related References: Cited from US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Jan 20, 2015:http://www.epa.gov/oppt/exposure/pubs/episuitedl.htm

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Physical Form or State
HERO ID:	3981013

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Results Value	solid
Results Details	not specified

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

Study Citation:	Lorz, P. M., Rowae, F. K., Enke, W., Jäckh, R., Bhargava, N., Hillesheim, W. (2007). Phthalic acid and derivatives. :132-180.
OECD Harmonized Template:	Physical Form or State
HERO ID:	679771

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Value	monoclinic crystals
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Physical Form or State
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Value	white crystals or fine white powder
Results Details	reported from two sources

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: National Toxicology Program, CAMEO Chemicals and Occupational Safety and Health Administration (OSHA)

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Physical Form or State
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Value	solid
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Human Metabolome Database (HMDB)

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Physical Form or State
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Value	crystalline powder
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: ILO International Chemical Safety Cards (ICSC)

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Physical Form or State
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Value	colorless crystals
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 14th Edition. John Wiley & Sons, Inc. New York, NY 2001., p. 875

Study Citation:	Rumble, J. R. (2018). Phthalic acid. :3-46.
OECD Harmonized Template:	Physical Form or State
HERO ID:	7274314

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Value	plates from water
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Elsevier, (2020). Reaxys: physical-chemical property data for phthalic acid. CAS Registry Number: 88-33-9..
OECD Harmonized Template:	Physical Form or State
HERO ID:	7274517

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details	white crystals

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Value reported by multiple primary sources in REAXYS.

Study Citation:	Elsevier, (2020). Reaxys: physical-chemical property data for phthalic acid. CAS Registry Number: 88-33-9..
OECD Harmonized Template:	Physical Form or State
HERO ID:	7274517

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details	colorless crystals

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Value reported by multiple primary sources in REAXYS.

Study Citation:	Elsevier, (2020). Reaxys: physical-chemical property data for phthalic acid. CAS Registry Number: 88-33-9..
OECD Harmonized Template:	Physical Form or State
HERO ID:	7274517

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details	yellow crystals

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Value reported by one primary source in REAXYS.

Study Citation:	Lorz, P. M., Rowae, F. K., Enke, W., Jäckh, R., Bhargava, N., Hillesheim, W. (2007). Phthalic acid and derivatives. :132-180.
OECD Harmonized Template:	Physical Form or State
HERO ID:	679771

EXTRACTION

Parameter	**Data**
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details	colorless, monoclinic crystals

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Melting Point
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Melting Point	Not Reported
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; sub cooled vapor pressure
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma; Not Reported; >99.5
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	enthalpy of fusion: 38.1 kJ/molMethod: Knudsen Effusion Mass Spectrometry (KEMS)combined with Differential Scanning Calorimetry (DSC)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information

Overall Quality Determination NEED TO FIX

* Related References: no references cited

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Melting Point
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Melting Point	479.9 - K
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; Not Reported; >99.5
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Knudsen Effusion Mass Spectrometry (KEMS) combined with Differential Scanning Calorimetry (DSC)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: no references cited

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Melting Point
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Melting Point	Not Reported
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; Not Reported; >99.5
Results Details Methods	Knudsen Effusion Mass Spectrometry (KEMS) combined with Differential Scanning Calorimetry (DSC)
Standard Deviation Results	Not Reported
Results Details	enthalpy of sublimation: 78.9 kJ/mol

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: no references cited

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Melting Point
HERO ID:	3981013

EXTRACTION

Parameter	**Data**
Melting Point	207 - °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; not specified; none
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Results Details Methods	not reported
Standard Deviation Results	not reported
Results Details	decomposes

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

Study Citation:	Elsevier, (2020). Reaxys: physical-chemical property data for phthalic acid. CAS Registry Number: 88-33-9..
OECD Harmonized Template:	Melting Point
HERO ID:	7274517

EXTRACTION

Parameter	**Data**
Melting Point	190 - 230 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not reported
Results Details	Measured conditions were not reported; 56 values were reported in Reaxys; 44 of these values were reported in the range of 190-230°C; 12 data points were outside the range. Decomposition reported in two entries.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Data range determined from multiple primary sources in REAXYS.

Study Citation:	Lorz, P. M., Rowae, F. K., Enke, W., Jäckh, R., Bhargava, N., Hillesheim, W. (2007). Phthalic acid and derivatives. :132-180.
OECD Harmonized Template:	Melting Point
HERO ID:	679771

EXTRACTION

Parameter	**Data**
Melting Point	191 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; sealed tube
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Converted into phthalic anhydride with the elimination of water at 210–211 C.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Monroe, K. P. (1920). Phthalic anhydride. II. The melting point of pure phthalic anhydride. the system: phthalic anhydride—phthalic acid. Journal of the Franklin Institute 189(1):103-104.
OECD Harmonized Template:	Melting Point
HERO ID:	5178041

EXTRACTION

Parameter	**Data**
Melting Point	208 ±2 °C
CASRN and Test Material	88-99-4; Phthalic anhydride
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; Very pure chemical prepared by re-sublimation in vacuo in the presence of P2O5 Notes: NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	eutectic temperature of phthalic anhydride and phthalic acid was determined to be 129.74°C

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed primary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Melting Point	410 - 412 F
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	decomposes
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Melting Point	230 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	decomposes
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination **High**

* Related References: PhysProp

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Melting Point	410 - 412 F
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Occupational Safety and Health Administration (OSHA)

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Melting Point	205 - 230 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination **High**

* Related References: Human Metabolome Database (HMDB)

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Melting Point	464.15 K
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; sealed tube
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Daubert, T.E., R.P. Danner. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis, 1989.

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Melting Point	210 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	converted into phthalic anhydride with the elimination of water
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA20: 182 (1992)

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	Melting Point
HERO ID:	679796

EXTRACTION

Parameter	**Data**
Melting Point	211 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	decomposes
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Melting Point	210 - 211 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	decomposes
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: SynQuest

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Melting Point	205 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	decomposes
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Melting Point	210 - 230 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Jean-Claude Bradley Open Melting Point Dataset

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Melting Point	204 - 209 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: LabNetwork

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Melting Point	210 - 211 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	decomposes
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Sigma-Aldrich

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Melting Point
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Melting Point	191 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	decomposes
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other			
Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Kaye & Laby

Study Citation:	Rumble, J. R. (2018). Phthalic acid. :3-46.
OECD Harmonized Template:	Melting Point
HERO ID:	7274314

EXTRACTION

Parameter	**Data**
Melting Point	207 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	decomposes
Standard Deviation Results	Not reported
Results Details	decomposes (reported under boiling point column)

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	U.S. EPA, (2020). Chemistry Dashboard Information for Phthalic Acid. 88-99-3..
OECD Harmonized Template:	Melting Point
HERO ID:	7274211

EXTRACTION

Parameter	**Data**
Melting Point	205 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Alfa Aesar (Chemical company)

Study Citation:	U.S. EPA, (2020). Chemistry Dashboard Information for Phthalic Acid. 88-99-3..
OECD Harmonized Template:	Melting Point
HERO ID:	7274211

EXTRACTION

Parameter	**Data**
Melting Point	210 - 230 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not reported
Results Details	Range 210-230°C

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Jean-Claude Bradley Open Melting Point Dataset

Study Citation:	U.S. EPA, (2020). Chemistry Dashboard Information for Phthalic Acid. 88-99-3..
OECD Harmonized Template:	Melting Point
HERO ID:	7274211

EXTRACTION

Parameter	**Data**
Melting Point	211 °C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: SynQuest Labs (Chemical company)

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Boiling Point
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Boiling Point	642.3 - K
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; estimated; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; sigma Aldrich; Not Reported; >99.5
Standard Deviation Results	Not Reported
Results Details	estimated using Nannoolal method

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Y. Nannoolal, J. Rarey, D. Ramjugernath and W. Cordes,Estimation of pure component properties Part 1. Estimation of thenormal boiling point of non-electrolyte organic compounds via groupcontributions and group interactions, Fluid Phase Equilib., 2004, 226,45–63.

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Boiling Point
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Boiling Point	642.5 - K
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; estimated; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; sigma Aldrich; Not Reported; >99.5
Standard Deviation Results	Not Reported
Results Details	estimated using Stein and Brown method

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: 7 S. E. Stein and R. L. Brown, Estimation of normal boiling pointsfrom group contributions, J. Chem. Inf. Model., 1994, 34, 581–587

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Boiling Point
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Boiling Point	Not Reported
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Standard Deviation Results	Not reported
Results Details	No quantitative data reported; two sources reported that phthalic acid decomposes. This is consistent with the melting point data.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: National Toxicology Program, IEHS, NIH. 1992. NTP Chemical Repository Database. RTP, NC and Lide and Milne(eds). Handbook of Data on Organic Compounds. Volume I. 3rd ed. CRC Press, Inc. Boca Raton ,FL. 1994., p. V1: 797.

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Density
HERO ID:	3981013

EXTRACTION

Parameter	**Data**
Density	2.18 -
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Density Type	specific gravity (density of a substance divided by the density of water)
System	not specified
Temperature	191°C
Standard Deviation Results	not reported
Results Details	not reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	Density
HERO ID:	679796

EXTRACTION

Parameter	**Data**
Density	1.593
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Density Type	density reported as specific gravity
System	NR
Temperature	4 deg C
Standard Deviation Results	NR
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Rumble, J. R. (2018). Phthalic acid. :3-46.
OECD Harmonized Template:	Density
HERO ID:	7274314

EXTRACTION

Parameter	**Data**
Density	2.18 - g/cm3
CASRN and Test Material	88-99-3; Not Reported
Confidentiality, Type, and Guideline	none; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	density
System	not specified
Temperature	191
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Elsevier, (2020). Reaxys: physical-chemical property data for phthalic acid. CAS Registry Number: 88-33-9..
OECD Harmonized Template:	Density
HERO ID:	7274517

EXTRACTION

Parameter	**Data**
Density	1.576 - 1.593 g/cm3
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not Reported
Standard Deviation Results	Not reported
Results Details	4 values were reported in Reaxys; 4 of these values were reported in the range of 1.576-1.593 g/cm3.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Data range determined from multiple primary sources in REAXYS.

Study Citation:	Lorz, P. M., Rowae, F. K., Enke, W., Jäckh, R., Bhargava, N., Hillesheim, W. (2007). Phthalic acid and derivatives. :132-180.
OECD Harmonized Template:	Density
HERO ID:	679771

EXTRACTION

Parameter	**Data**
Density	1.593 g/cm3
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	15°C
Standard Deviation Results	Not Reported
Results Details	reported at 15°C

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Myhre, L., C.E., Nielsen, C. J. (2004). Optical properties in the UV and visible spectral region of organic acids relevant to tropospheric aerosols. Atmospheric Chemistry and Physics 4(7):1759-1769.
OECD Harmonized Template:	Density
HERO ID:	3339378

EXTRACTION

Parameter	**Data**
Density	0.99815 - 0.9985 g/cm3
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	293 K
Standard Deviation Results	1x10-6 g/cm3
Results Details	0.99815 at pH 2.75 and 0.99850 at pH 2.67 at 293K and concentration of 0.07 and 0.11 wt%, respectively. Measured with a Density/Specific Gravity/Concentration Meter, DMA 5000.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Density
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Density	1.593 - units not given
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	68 deg F
Standard Deviation Results	Not reported
Results Details	reported as 1.593 at 68 deg F and 1.593 from two sources

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	Units not reported but expected to be g/cm3.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: CAMEO Chemicals and Occupational Safety and Health Administration (OSHA)

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Density
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Density	1.593 - g/cm3
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	15°C
Standard Deviation Results	Not reported
Results Details	1.593 g/cu cm at 15°C

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Gerhartz, W. (exec ed.). Ullmann's Encyclopedia of Industrial Chemistry. 5th ed.Vol A1: Deerfield Beach, FL: VCH Publishers, 1985 to Present., p. VA20: 182 (1992)

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Density
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Density	1.6 units not given
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not Reported
Standard Deviation Results	Not reported
Results Details	reported as Relative density (water=1): 1.6

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	Units not reported but expected to be g/cm3.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: ILO International Chemical Safety Cards (ICSC).

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Density
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Density	1.593 g/cm3
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not Reported
Standard Deviation Results	Not reported
Results Details	reported as 1.593 g/mL

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Alfa Aesar

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Density
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Density	1.593 g/cm3
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not Reported
Standard Deviation Results	Not reported
Results Details	reported as 1.593 g/mL

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: SynQuest

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Density
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Density	1.593 g/cm3
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	20°C
Standard Deviation Results	Not reported
Results Details	reported as 1.593 g/mL; source no longer updated

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Kaye & Laby

Study Citation:	Rumble, J. R. (2018). Phthalic acid. :3-46.
OECD Harmonized Template:	Density
HERO ID:	7274314

EXTRACTION

Parameter	**Data**
Density	2.18 g/cm3
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; None
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	191°C
Standard Deviation Results	Not reported
Results Details	Reported as 2.18 g/cm3 at 191°C

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Density
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Density	5.7
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Not reported
Temperature	Not Reported
Standard Deviation Results	Not reported
Results Details	Relative vapor density (air=1)

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: ILO International Chemical Safety Cards (ICSC)

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Density
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Density	5.73
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Not reported
Temperature	Not Reported
Standard Deviation Results	Not reported
Results Details	Air = 1

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: National Fire Protection Association. Fire Protection Guide on Hazardous Materials. 6th ed. Boston, Mass.: National Fire Protection Association, 1975., p. 325M-119

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	1.68E-3 - Pa
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; sub cooled vapor pressure
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; solid; >99.5%
Temperature	Not Reported
System	TA instruments Q200 Differential Scanning Calorimeter
Standard Deviation Results	0.84E-10
Results Details	Method: Knudsen Effusion Mass Spectrometry (KEMS)combined with Differential Scanning Calorimetry (DSC)reported as sub-cooled liquid vapor pressure

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

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Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EVALUATION

Domain	Metric	Rating	Comments

* Related References: no references cited

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	1.77 x10-5 - Pa
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; solid; >99.5%
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Method: Knudsen Effusion Mass Spectrometry (KEMS)combined with Differential Scanning Calorimetry (DSC)reported as solid state vapour pressure

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: no references cited

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	6.17 E-5 - Pa
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; sub cooled liquid vapor pressure
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; liquid; >99.5%
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Nannoolal/Nannoolal methodratio of estimated to measured subcooled liquid vapor pressure: 3.7E-2 Pa

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Y. Nannoolal, J. Rarey, D. Ramjugernath and W. Cordes,Estimation of pure component properties Part 1. Estimation of thenormal boiling point of non-electrolyte organic compounds via groupcontributions and group interactions, Fluid Phase Equilib., 2004, 226,45–63.29 Y. Nannoolal, J. Rarey and D. Ramjugernath,contributions and group interactions, Fluid Phase Equilib., 2008, 269,117–133

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; Not Reported; >99.5%
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Estimated enthalpy of vaporization uding the Nannoolal/Nannoolal method: 118 kJ/mol

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Y. Nannoolal, J. Rarey, D. Ramjugernath and W. Cordes,Estimation of pure component properties Part 1. Estimation of thenormal boiling point of non-electrolyte organic compounds via groupcontributions and group interactions, Fluid Phase Equilib., 2004, 226,45–63.Y. Nannoolal, J. Rarey and D. Ramjugernath, Part 3. Estimation ofthe vapor pressure of non-electrolyte organic compounds via group contributions and group interactions, Fluid Phase Equilib., 2008, 269,117–133

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; Not Reported; >99.5%
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Estimated enthalpy of vaporization using the Myrdal and Yalkowsky/Stein and Brownmethod method: 92 kJ/mol

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: P. B. Myrdal and S. H. Yalkowsky, Estimating pure componentvapour pressures of complex organic molecules, Ind. Eng. Chem. Res.,1997, 36, 2494–2499. S. E. Stein and R. L. Brown, Estimation of normal boiling pointsfrom group contributions, J. Chem. Inf. Model., 1994, 34, 581–587.

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; sub cooled vapor pressure
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; Not Reported; >99.5%
Temperature	Not Reported
System	TA instruments Q200 Differential Scanning Calorimeter
Standard Deviation Results	Not Reported
Results Details	enthalpy of vaporization: 40.7 +/- 8.5 kJ/molMethod: Knudsen Effusion Mass Spectrometry (KEMS)combined with Differential Scanning Calorimetry (DSC)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: no references cited

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	4.95 E-7 - Pa
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; sub cooled liquid vapor pressure
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; liquid; >99.5%
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Moller/Nannoolal methodratio of estimated to measured subcooled liquid vapor pressure: 2.9E-4 Pa

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: B. Moller, J. Rarey and D. Ramjugernath, Estimation of the vapourpressure of non-electrolyte organic compounds via group contributions and group interactions, J. Mol. Liq., 2008, 143, 52–63.Y. Nannoolal, J. Rarey, D. Ramjugernath and W. Cordes,Estimation of pure component properties Part 1. Estimation of thenormal boiling point of non-electrolyte organic compounds via groupcontributions and group interactions, Fluid Phase Equilib., 2004, 226,45–63.

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	1.68E-3 - Pa
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; sub cooled liquid vapor pressure
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; liquid; >99.5%
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	KEMS

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: no reference cited

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; Not Reported; >99.5%
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Estimated enthalpy of vaporization using the KEMSmethod: 41 kJ/mol

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: no references cited

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	Not Reported
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; Not Reported; >99.5%
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Estimated enthalpy of vaporization uding the Moller/Nannoolal method: 158 kJ/mol

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: B. Moller, J. Rarey and D. Ramjugernath, Estimation of the vapourpressure of non-electrolyte organic compounds via group contributions and group interactions, J. Mol. Liq., 2008, 143, 52–63Y. Nannoolal, J. Rarey, D. Ramjugernath and W. Cordes,Estimation of pure component properties Part 1. Estimation of thenormal boiling point of non-electrolyte organic compounds via groupcontributions and group interactions, Fluid Phase Equilib., 2004, 226,45–63.

Study Citation:	Booth, A. M., Bannan, T., McGillen, M. R., Barley, M. H., Topping, D. O., McFiggans, G., Percival, C. J. (2012). The role of ortho, meta, para isomerism in measured solid state and derived sub-cooled liquid vapour pressures of substituted benzoic acids. RSC Advances 2(10):4430-4443.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6817917

EXTRACTION

Parameter	**Data**
Vapor Pressure	4.76E-3 - Pa
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; sub cooled liquid vapor pressure
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Sigma Aldrich; liquid; >99.5%
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Myrdal and Yalkowsky/Steinand Brown methodratio of estimated to measured subcooled liquid vapor pressure: 2.8 Pa

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: P. B. Myrdal and S. H. Yalkowsky, Estimating pure componentvapour pressures of complex organic molecules, Ind. Eng. Chem. Res.,1997, 36, 2494–2499. S. E. Stein and R. L. Brown, Estimation of normal boiling pointsfrom group contributions, J. Chem. Inf. Model., 1994, 34, 581–587

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	3981013

EXTRACTION

Parameter	**Data**
Vapor Pressure	6.36x10-7 - mm Hg
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Temperature	25°C
System	not reported
Standard Deviation Results	not reported
Results Details	not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Vapor Pressure	6.36e-7 torr
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 6.36e-07 mmHg

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: EPA DSSTox

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Vapor Pressure	6.36e-7 torr
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 6.36X10-7 mm Hg at 25°C

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination **High**

* Related References: Daubert, T.E., R.P. Danner. Physical and Thermodynamic Properties of Pure Chemicals Data Compilation. Washington, D.C.: Taylor and Francis, 1989.

Study Citation:	U.S. EPA, (2020). Chemistry Dashboard Information for Phthalic Acid. 88-99-3..
OECD Harmonized Template:	Vapor Pressure
HERO ID:	7274211

EXTRACTION

Parameter	**Data**
Vapor Pressure	6.36e-7 torr
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not reported
Standard Deviation Results	Not reported
Results Details	reported as 6.36e-7 mmHg

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: PhysProp

Study Citation:	Elsevier, (2020). Reaxys: physical-chemical property data for phthalic acid. CAS Registry Number: 88-33-9..
OECD Harmonized Template:	logKow
HERO ID:	7274517

EXTRACTION

Parameter	**Data**
log k_{ow}	0.26
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	logKow
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
log k_{ow}	0.73
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Same result of 0.73, 0.73 (logP), log kow=0.73, 0.73 reported 4 times with same reference source.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society., 1995., p. 38

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	logKow
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
log k_{ow}	0.304
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Not reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: LabNetwork

Study Citation:	U.S. EPA, (2020). Chemistry Dashboard Information for Phthalic Acid. 88-99-3..
OECD Harmonized Template:	logKow
HERO ID:	7274211

EXTRACTION

Parameter	**Data**
log k_{ow}	0.730
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: PhysPropNCCT

Study Citation:	Box, K. J., Völgyi, G., Baka, E., Stuart, M., Takács-Novák, K., Comer, A., J.E. (2006). Equilibrium versus kinetic measurements of aqueous solubility, and the ability of compounds to supersaturate in solution — A validation study. Journal of Pharmaceutical Sciences 95(6):1298-1307.
OECD Harmonized Template:	Water Solubility
HERO ID:	6968979

EXTRACTION

Parameter	**Data**
Water Solubility	5950 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	no; Sigma (Poole, Dorset, UK); Solid; analytical grade
Temperature	25.0°C
System	GLpKa titrator with a pH electrode (combination Ag–AgCl), and a D-PAS spectrometer fitted with a bifurcated fiber optic dip probe. Titrations were performed in 0.15 M KCl under argon atmosphere, at 25±1 deg C, using 0.5 M HCL and 0.5 M KOH solutions.
pH	0.5
Results Details Method	shake flask method; heterogeneous system; 48 hour saturation time at 25±0.1 deg C; 9-21 data points measured at maximum wavelength of 275 nm
Standard Deviation Results	±200 mg/L
Results Details	Intrinsic solubility reported as 5950±200 µg/mL or 35800±1000 µM. The intrinsic solubility is the concentration of unionized species at the pH where the compound is fully unionized.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Box, K. J., Völgyi, G., Baka, E., Stuart, M., Takács-Novák, K., Comer, A., J.E. (2006). Equilibrium versus kinetic measurements of aqueous solubility, and the ability of compounds to supersaturate in solution — A validation study. Journal of Pharmaceutical Sciences 95(6):1298-1307.
OECD Harmonized Template:	Water Solubility
HERO ID:	6968979

EXTRACTION

Parameter	**Data**
Water Solubility	5330 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	no; Sigma (Poole, Dorset, UK); Solid; analytical grade
Temperature	25°C
System	GLpKa titrator with a pH electrode (combination Ag–AgCl), and a D-PAS spectrometer fitted with a bifurcated fiber optic dip probe. Titrations were performed in 0.15 M KCl under argon atmosphere, at 25±1 deg C, using 0.5 M HCL and 0.5 M KOH solutions.
pH	Not reported
Results Details Method	Chasing Equilibrium method; the equilibriumsolubility is actively sought by changing the concentration of the neutral form by adding HCl or KOH titrants and monitoring the rate of change of pH due to precipitation or dissolution.
Standard Deviation Results	±47 mg/L
Results Details	Intrinsic solubility reported as 5330±47 µg/mL or 32080±287 µM. The intrinsic solubility is the concentration of unionized species at the pH where the compound is fully unionized.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Elsevier, (2020). Reaxys: physical-chemical property data for phthalic acid. CAS Registry Number: 88-33-9..
OECD Harmonized Template:	Water Solubility
HERO ID:	7274517

EXTRACTION

Parameter	**Data**
Water Solubility	6944 - 7958 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	145 values were reported in Reaxys; 9 of these values were reported in the range of 6944-7958 mg/L at 25°C in H2O; other data points were measured at a lower or higher temperature or in solutions with other chemicals. Actual reported values:25°C 647.906 g/L (decimal typo?)25°C 7.95763 g/L25°C 6.99407 g/L25°C 7.01069 g/L25°C 7.04391 g/L25°C 6.94423 g/L 25°C 0.07613 mol%25°C 0.0425 mol/kg25°C 0.7014 g/100g

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

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Study Citation:	Elsevier, (2020). Reaxys: physical-chemical property data for phthalic acid. CAS Registry Number: 88-33-9..
OECD Harmonized Template:	Water Solubility
HERO ID:	7274517

		EVALUATION	
Domain	Metric	Rating	Comments

* Related References: Data range determined from multiple primary sources in REAXYS.

Study Citation:	Han, N. Y., Zhu, L., Wang, L. S., Fu, R. N. (1999). Aqueous solubility of m-phthalic acid, o-phthalic acid and p-phthalic acid from 298 to 483 K. Separation and Purification Technology 16(2):175-180.
OECD Harmonized Template:	Water Solubility
HERO ID:	6826968

EXTRACTION

Parameter	**Data**
Water Solubility	6940 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	Water; NR; NR; NR
Radiolabel, Source, State, and Purity	no; NR; Solid; >99.98% Notes: analytical-grade
Temperature	298.15 K
System	equilibrium cell immersed in an air bath (temperature controlled within ±0.2°C by a thermocouple), electric rocking system used to agitate the cell.
pH	Not reported
Results Details Method	The mass of sampling was weighed using an electronic balance (accuracy ±0.0001 g) and the solubility of the sample was determined by titrating with sodium hydroxide standard solution.
Standard Deviation Results	Not reported
Results Details	Reported as 0.7522x10+3 mole fraction at 298.15 K. A trend of increasing solubility with temperature is observed.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard. Some study details such as pH were not reported.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Han, N. Y., Zhu, L., Wang, L. S., Fu, R. N. (1999). Aqueous solubility of m-phthalic acid, o-phthalic acid and p-phthalic acid from 298 to 483 K. Separation and Purification Technology 16(2):175-180.
OECD Harmonized Template:	Water Solubility
HERO ID:	6826968

EXTRACTION

Parameter	**Data**
Water Solubility	9850 - 1,812,000 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	Water; NR; NR; NR
Radiolabel, Source, State, and Purity	no; NR; Solid; >99.98% Notes: analytical-grade
Temperature	308.15 to 428.15 K
System	equilibrium cell immersed in an air bath (temperature controlled within ±0.2°C by a thermocouple), electric rocking system used to agitate the cell.
pH	Not reported
Results Details Method	The mass of sampling was weighed using an electronic balance (accuracy ±0.0001 g) and the solubility of the sample was determined by titrating with sodium hydroxide standard solution.
Standard Deviation Results	Not reported
Results Details	Reported as 1.068x10+3 to 196.5x10+3 mole fraction at 10 temperatures from 308.15 to 428.15 K. A trend of increasing solubility with temperature is observed.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Water Solubility
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Water Solubility	6250 - 7010 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	6 values were reported as 7010 mg/L, 6965 mg/L, 7.01 mg/mL, 0.625 g/100 mL at 25°C , 0.04 Molar and for 1 g in 160 mL water

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Water Solubility
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Water Solubility	< 1000 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	68°F
System	Not Reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as less than 1 mg/mL at 68 deg F

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992.

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	Water Solubility
HERO ID:	679796

EXTRACTION

Parameter	**Data**
Water Solubility	7000 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 0.7 g/100g water at 25 deg C and reported as 19.0 g/100 g water at 100 deg C and 200 g/100g at 150 deg C

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Rumble, J. R. (2018). Aqueous solubility and Henry's law constants of organic compounds. :5-148 - 5-177.
OECD Harmonized Template:	Water Solubility
HERO ID:	5932745

EXTRACTION

Parameter	**Data**
Water Solubility	4658 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	10°C
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 0.464 mass%; 4.66 g/kg H2O; converted using CRC handbook's reported water density at 10 C.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Apelblat, A., Manzurola, E., and Bala!, N. A., f. Chem. Thermodynamics 38, 565, 2006.

Study Citation:	Rumble, J. R. (2018). Aqueous solubility and Henry's law constants of organic compounds. :5-148 - 5-177.
OECD Harmonized Template:	Water Solubility
HERO ID:	5932745

EXTRACTION

Parameter	**Data**
Water Solubility	7219 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 0.719 mass%; 7.24 g/kg H2O; converted using CRC handbook's reported water density at 25 C.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Apelblat, A., Manzurola, E., and Bala!, N. A., f. Chem. Thermodynamics 38, 565, 2006.

Study Citation:	Rumble, J. R. (2018). Aqueous solubility and Henry's law constants of organic compounds. :5-148 - 5-177.
OECD Harmonized Template:	Water Solubility
HERO ID:	5932745

EXTRACTION

Parameter	**Data**
Water Solubility	36282 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	65°C
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 3.57 mass%; 37.0 g/kg H2O; converted using CRC handbook's reported water density at 65 C.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Apelblat, A., and Manzurola, E., f. Chem. Thermodynamics 21, 1005, 1989.

Study Citation:	Rumble, J. R. (2018). Aqueous solubility and Henry's law constants of organic compounds. :5-148 - 5-177.
OECD Harmonized Template:	Water Solubility
HERO ID:	5932745

EXTRACTION

Parameter	**Data**
Water Solubility	17686 mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	50°C
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 1.76 mass%; 17.9 g/kg H2O; converted using CRC handbook's reported water density at 50 C.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Apelblat, A., Manzurola, E., and Bala!, N. A., f. Chem. Thermodynamics 38, 565, 2006.

Study Citation:	Rumble, J. R. (2018). Phthalic acid. :3-46.
OECD Harmonized Template:	Water Solubility
HERO ID:	7274314

EXTRACTION

Parameter	**Data**
Water Solubility	Not Reported
CASRN and Test Material	88-99-3; Not Reported
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	sl in water, ether; insol chl; s EthOH

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Low

Study Citation:	U.S. EPA, (2020). Chemistry Dashboard Information for Phthalic Acid. 88-99-3..
OECD Harmonized Template:	Water Solubility
HERO ID:	7274211

EXTRACTION

Parameter	**Data**
Water Solubility	6994 - mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 0.0421 mol/L

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: PhysProp

Study Citation:	U.S. EPA, (2020). Chemistry Dashboard Information for Phthalic Acid. 88-99-3..
OECD Harmonized Template:	Water Solubility
HERO ID:	7274211

EXTRACTION

Parameter	**Data**
Water Solubility	1290 - mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 0.00776 mol/L

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Tetko et al. J. Chem. Inf. and Comp. Sci. 41.6 (2001): 1488-1493

Study Citation:	U.S. EPA, (2020). Chemistry Dashboard Information for Phthalic Acid. 88-99-3..
OECD Harmonized Template:	Water Solubility
HERO ID:	7274211

EXTRACTION

Parameter	**Data**
Water Solubility	7094 - mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 0.0427 mol/L

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Kovdienko, et. al. Molecular informatics 29.5 (2010): 394-406.

Study Citation:	U.S. EPA, (2020). Chemistry Dashboard Information for Phthalic Acid. 88-99-3..
OECD Harmonized Template:	Water Solubility
HERO ID:	7274211

EXTRACTION

Parameter	**Data**
Water Solubility	5383 - mg/L
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 0.0324 mol/L

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Boobier, et. al. "Can human experts predict solubility better than computers?"

Study Citation:	Lorz, P. M., Rowae, F. K., Enke, W., Jäckh, R., Bhargava, N., Hillesheim, W. (2007). Phthalic acid and derivatives. :132-180.
OECD Harmonized Template:	Flash Point
HERO ID:	679771

EXTRACTION

Parameter	**Data**
Flash Point	168 C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Not reported
Standard Deviation Results	Not reported
Results Details	Not reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Flash Point
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Flash Point	334 F
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Not reported
Standard Deviation Results	Not reported
Results Details	Two sources reported 334°F

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Occupational Safety and Health Administration (OSHA) and Fire Protection Guide to Hazardous Materials. 13 ed. Quincy, MA: NFPA, 2002., p. 325-99

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	Flash Point
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
Flash Point	168 C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; closed cup
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Not Reported
Standard Deviation Results	Not reported
Results Details	Reported as 334°F (168°C) and 168°C c.c.

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: ILO International Chemical Safety Cards (ICSC) and Fire Protection Guide to Hazardous Materials. 13 ed. Quincy, MA: National Fire Protection Association, 2002., p. 325-99

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Flash Point
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Flash Point	168 C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Not reported
Standard Deviation Results	Not reported
Results Details	Not reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: Alfa Aesar

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Flash Point
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Flash Point	168 C
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	none; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Not reported
Standard Deviation Results	Not reported
Results Details	Not reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: Alfa Aesar

Study Citation:	Rumble, J. R. (2018). Flammability of chemical substances. :16-16 - 16-32.
OECD Harmonized Template:	Flash Point
HERO ID:	6655446

EXTRACTION

Parameter	**Data**
Flash Point	168 C
CASRN and Test Material	Not Reported; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a known data-collection, prepared by experts in the field.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Box, K. J., Völgyi, G., Baka, E., Stuart, M., Takács-Novák, K., Comer, A., J.E. (2006). Equilibrium versus kinetic measurements of aqueous solubility, and the ability of compounds to supersaturate in solution — A validation study. Journal of Pharmaceutical Sciences 95(6):1298-1307.
OECD Harmonized Template:	pKa
HERO ID:	6968979

EXTRACTION

Parameter	**Data**
pK_a	2.70
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	no; Sigma (Poole, Dorset, UK); Solid; analytical grade
Temperature	25°C
System	Not reported
pH	Not reported
Results Details Method	0.15 M ionic strength
Standard Deviation Results	Not reported
Results Details	First pKa 2.70 (acid)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Box, K. J., Völgyi, G., Baka, E., Stuart, M., Takács-Novák, K., Comer, A., J.E. (2006). Equilibrium versus kinetic measurements of aqueous solubility, and the ability of compounds to supersaturate in solution — A validation study. Journal of Pharmaceutical Sciences 95(6):1298-1307.
OECD Harmonized Template:	pKa
HERO ID:	6968979

EXTRACTION

Parameter	**Data**
pK_a	4.84
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	no; Sigma (Poole, Dorset, UK); Solid; analytical grade
Temperature	25°C
System	Not reported
pH	Not reported
Results Details Method	0.15 M ionic strength
Standard Deviation Results	Not reported
Results Details	Second pKa 4.84 (acid)

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Elsevier, (2020). Reaxys: physical-chemical property data for phthalic acid. CAS Registry Number: 88-33-9..
OECD Harmonized Template:	pKa
HERO ID:	7274517

EXTRACTION

Parameter	**Data**
pK_a	2.36 - 3.11
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	potentiometric
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	199 values were reported in Reaxys; 11 values were reported in the range of 2.36-5.08 for pka1 at 25°C using potentiometric method; 1 value was reported as 2.9 using spectrophotometric method at 25 deg C; other values were performed with other chemicals, at other temperatures, unreported temperature or unreported method.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Data range determined from multiple primary sources in REAXYS.

Study Citation:	Elsevier, (2020). Reaxys: physical-chemical property data for phthalic acid. CAS Registry Number: 88-33-9..
OECD Harmonized Template:	pKa
HERO ID:	7274517

EXTRACTION

Parameter	**Data**
pK_a	4.61 - 5.42
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	potentiometric
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	199 values were reported in Reaxys; 10 values were reported at 25°C using potentiometric method in the range of 4.61-5.42 for pka2; 1 value was reported as 5.25 using spectrophotometric method at 25 C; 22 values were reported at higher/lower than 25°C or unreported temperature or method.

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Data range determined from multiple primary sources in REAXYS.

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4319 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	0 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4326 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	0 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4324 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	0 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0005
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4323 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	0 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4177 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	5 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0010
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4091 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	10 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0009
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4043 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	15 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4041 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	20 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0009
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4150 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	30 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4077 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4259 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	35 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0010
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.5522 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	40 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0009
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4613 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	45 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0010
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4840 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	50 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.5108 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	55 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0011
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.5416 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	60 deg C
System	Series A solution had a buffer ratio of 1.0057 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0014
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and emf recording instruments
Standard Deviation Results	0.0009
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4182 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	5 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4093 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	10 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4050 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	15 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4041 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	20 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4079 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4154 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	30 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4269 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	35 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4423 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	40 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4615 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	45 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0006
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4848 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	50 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.5116 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	55 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0006
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.5403 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	60 deg C
System	Series B solution had a buffer ratio of 1.5070 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0035
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0005
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4095 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	10 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0005
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4178 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	5 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0004
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4053 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	15 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4047 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	20 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0006
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4085 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0006
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4165 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	30 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0011
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4278 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	35 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4426 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	40 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4857 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	50 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0011
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4616 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	45 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0006
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.5128 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	55 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.5414 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	60 deg C
System	Series C solution had a buffer ratio of 2.0005 and a chloride-acid phthalate ratio, KC1/KHPh, of 1.0006
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0005
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4184 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	5 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0006
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4103 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	10 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0008
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4060 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	15 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0012
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4053 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	20 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0006
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4090 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0010
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4160 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	30 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0006
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4276 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	35 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4423 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	40 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0009
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4849 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	50 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0005
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.5137 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	55 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.4625 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	45 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0005
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. old pre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Acree, S. F. (1945). Second dissociation constant of o-phthalic acid and related pH values of phthalate buffers from 0 degrees to 60 degrees C. 35:381-416.
OECD Harmonized Template:	pKa
HERO ID:	6815698

EXTRACTION

Parameter	**Data**
pK_a	5.5418 -
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; Measurements of electromotive forces with hydrogen electrodes and Silver-silver-chloride electrodes
Solvent, Reactivity, Storage, and Stability	high grade and distilled water of pH 6.7 to 7.3; NR; prepared in CO2-free atmosphere and deaerated by hydrogen gas; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	60 deg C
System	Series D solution had a buffer ratio of 2.0223 and a chloride-acid phthalate ratio, KC1/KHPh, of 0.1858
pH	4.87-5.72
Results Details Method	cells, bubble tubes, thermostat, and the emf recording instruments
Standard Deviation Results	0.0007
Results Details	second dissociation constant = log K2 = -2175.83/T+9.55095-0.025694T, where T = t deg C+273.16

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features(e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question,and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate (e.g. oldpre-guideline study using appropriate testing approach).
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Hamer, W. J., Pinching, G. D., Acree, S. F. (1945). First dissociation constant of o-phthalic acid and related pHvalues of phthalate buffers from 0 degrees to 60 degrees C. 35:539-564.
OECD Harmonized Template:	pKa
HERO ID:	6957658

EXTRACTION

Parameter	Data
pK_a	2.9343 - 2.9513
CASRN and Test Material	NR; o-phthalic acid
Confidentiality, Type, and Guideline	No; experimental; potential difference measured between electrodes in solution
Solvent, Reactivity, Storage, and Stability	Aqueous solutions of phthalic acid, potassium phthalate, and potassium chloride; NR; NR; NR
Radiolabel, Source, State, and Purity	NA; NR; aqueous solution; Recrystallized 3 times from distilled water and extracted with benzene in a Soxhlet extractor Notes: prepared in a CO2-free atmosphere
Temperature	0-60 deg C
System	Apparatus included the cells, bubble tubes, thermostat, and emf recording instruments.
pH	2.70 to 3.26
Results Details Method	potential difference measured between hydrogen electrodes and silver-silver-chloride electrodes; emf measured by means of a calibrated potentiometer with galvanometer and standard cell
Standard Deviation Results	NR
Results Details	first dissociation constant = log K1 = -561.57/T+1.2843-0.0078833T, where T = 273.16

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard (pre-guideline; study published in 1945) but is expected to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information

Overall Quality Determination High

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Study Citation:	Hamer, W. J., Pinching, G. D., Acree, S. F. (1945). First dissociation constant of o-phthalic acid and related pHvalues of phthalate buffers from 0 degrees to 60 degrees C. 35:539-564.
OECD Harmonized Template:	pKa
HERO ID:	6957658

EVALUATION

Domain	Metric	Rating	Comments

Study Citation:	NCBI, (2020). PubChem Database: Compound Summary: Phthalic acid.
OECD Harmonized Template:	pKa
HERO ID:	7274473

EXTRACTION

Parameter	**Data**
pK_a	2.76
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	Not reported
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	reported as pKa1 = 2.76; pKa2 = 4.92 at 25°C

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Serjeant EP, Dempsey B; IUPAC Chemical Data Series No 23 NY, NY: Pergamon Press (1979)

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	pKa
HERO ID:	679796

EXTRACTION

Parameter	**Data**
pK_a	2.95
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	pk1 in aqueous solution
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45.
OECD Harmonized Template:	pKa
HERO ID:	679796

EXTRACTION

Parameter	**Data**
pK_a	5.41
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	pk2 in aqueous solution
pH	Not reported
Results Details Method	Not reported
Standard Deviation Results	Not reported
Results Details	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Partanen, J. I., Covington, A. K. (2006). Re-evaluation of the first and second stoichiometric dissociation constants of phthalic acid at temperatures from (0 to 60) degrees C in aqueous phthalate buffer solutions with or without potassium chloride. 1. Estimation of the parameters for the Huckel model activity coefficient equations for calculation of the second dissociation constant. Journal of Chemical and Engineering Data 51(3):777-784.
OECD Harmonized Template:	pKa
HERO ID:	6816218

EXTRACTION

Parameter	**Data**
pK_a	5.399
CASRN and Test Material	Not Reported; phthalic acid
Confidentiality, Type, and Guideline	no; calculation; Estimation of the Parameters for the Huckel Model Activity Coefficient Equations
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	results reported as 2.92-4.02X10^6 Ka2 at 0-60°C; -log pKa2 = log (10^6 Ka2 value) x (10^-6)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Partanen, J. I., Covington, A. K. (2006). Re-evaluation of the first and second stoichiometric dissociation constants of phthalic acid at temperatures from (0 to 60) degrees C in aqueous phthalate buffer solutions with or without potassium chloride. 2. Estimation of parameters for the model for the first dissociation constant and tests and use of the resulting activity coefficient equations. Journal of Chemical and Engineering Data 51(6):2065-2073.
OECD Harmonized Template:	pKa
HERO ID:	6816224

EXTRACTION

Parameter	**Data**
pK_a	2.9404 (at 20°C) - 2.9481 (at 25°C)
CASRN and Test Material	Not Reported; phthalic acid
Confidentiality, Type, and Guideline	no; calculation; Estimation of Parameters for the Model for the First Dissociation Constant
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	20, 25°C
System	thermodynamic value of first dissociation constant (- log pKa1); least-squares fitting of experimental data from previous study
pH	not reported
Results Details Method	not applicable
Standard Deviation Results	0.0002-0.0003
Results Details	Ka1 range of results reported 0.939X10^3 at 60°C to 1.197X10^3 at 0°C; -log pKa1 = log (10^3 Ka1 value) x (10^-3)

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Calculated data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	High	The model had a defined, unambiguous endpoint.

Overall Quality Determination High

Study Citation:	Rumble, J. R., Lide, D. R., Bruno, T. J. (2018). Dissociation constants of organic acids and bases. :5-105-5-114.
OECD Harmonized Template:	pKa
HERO ID:	10633660

EXTRACTION

Parameter	**Data**
pK_a	5.432 -
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	pKa 2

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was us
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: Seven references cited but none were specific to the test substance.

Study Citation:	Rumble, J. R., Lide, D. R., Bruno, T. J. (2018). Dissociation constants of organic acids and bases. :5-105-5-114.
OECD Harmonized Template:	pKa
HERO ID:	10633660

EXTRACTION

Parameter	**Data**
pK_a	2.943 -
CASRN and Test Material	88-99-3; phthalic acid
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	pKa 1

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: Seven references cited but none were specific to the test substance.

Study Citation:	Singh, A. K., Ghosh, J. C. (1985). 1st Dissociation-constant of ortho-phthalic acid from 283.15 to 323.15-K. Journal of the Indian Chemical Society 62(2):158-160.
OECD Harmonized Template:	pKa
HERO ID:	6815331

EXTRACTION

Parameter	**Data**
pK_a	2.930 - 2.996
CASRN and Test Material	Not Reported; o-phthalic acid
Confidentiality, Type, and Guideline	None; experimental; Modified Davies equation applied to measured data
Solvent, Reactivity, Storage, and Stability	double distilled water; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; 99.95% purity Notes: General Reagent (G.R.)
Temperature	283.15 to 323.15K
System	Thermostat and potentiometric assembly and measurement of electromagnetic fields and molalities were measured
pH	NR
Results Details Method	EMF values collected in abs volt and used in calculations
Standard Deviation Results	+/-0.0007 to 0.0021
Results Details	pK1 are 2.930 at 283.15K to 2.996 (or 2.997 from cell C2) at 323.15K

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is non-standard but is expected to be appropriate; however, pH conditions were not explicitly reported.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

Study Citation:	Tam, K. Y., Takacs-Novak, K. (1999). Multiwavelength spectrophotometric determination of acid dissociation constants: Past II. First derivative vs. target factor analysis. Pharmaceutical Research 16(3):374-381.
OECD Harmonized Template:	pKa
HERO ID:	2790730

EXTRACTION

Parameter	**Data**
pK_a	2.70 -
CASRN and Test Material	88-99-3; Phthalic Acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
System	Target Factor Analysis
pH	2.70 +/- 0.01
Results Details Method	0.15 M ionic strength
Standard Deviation Results	0.01
Results Details	pKa1; compared to pH metric 2.74 +/- 0.02

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Tam, K. Y., Takacs-Novak, K. (1999). Multiwavelength spectrophotometric determination of acid dissociation constants: Past II. First derivative vs. target factor analysis. Pharmaceutical Research 16(3):374-381.
OECD Harmonized Template:	pKa
HERO ID:	2790730

EXTRACTION

Parameter	**Data**
pK_a	2.74 -
CASRN and Test Material	88-99-3; Phthalic Acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
System	First derivative spectrophotometry
pH	2.74 +/- 0.06
Results Details Method	0.15 M ionic strength
Standard Deviation Results	0.06
Results Details	pKa1; compared to pH metric 2.74 +/- 0.02

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Tam, K. Y., Takacs-Novak, K. (1999). Multiwavelength spectrophotometric determination of acid dissociation constants: Past II. First derivative vs. target factor analysis. Pharmaceutical Research 16(3):374-381.
OECD Harmonized Template:	pKa
HERO ID:	2790730

EXTRACTION

Parameter	**Data**
pK_a	4.87 -
CASRN and Test Material	88-99-3; Phthalic Acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
System	First derivative spectrophotometry
pH	4.87 +/- 0.03
Results Details Method	0.15 M ionic strength
Standard Deviation Results	0.03
Results Details	pKa2, compared to pH-metric 4.84 +/- 0.01

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Tam, K. Y., Takacs-Novak, K. (1999). Multiwavelength spectrophotometric determination of acid dissociation constants: Past II. First derivative vs. target factor analysis. Pharmaceutical Research 16(3):374-381.
OECD Harmonized Template:	pKa
HERO ID:	2790730

EXTRACTION

Parameter	**Data**
pK_a	4.86 -
CASRN and Test Material	88-99-3; Phthalic Acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
System	Target Factor Analysis
pH	4.86 +/- 0.01
Results Details Method	0.15 M ionic strength
Standard Deviation Results	0.01
Results Details	pKa2, compared to pH-metric 4.84 +/- 0.01

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

Study Citation:	Tummanapelli, A. K., Vasudevan, S. (2015). Estimating successive pKa values of polyprotic acids from ab initio molecular dynamics using metadynamics: the dissociation of phthalic acid and its isomers. Physical Chemistry Chemical Physics 17(9):6383-6388.
OECD Harmonized Template:	pKa
HERO ID:	4278044

EXTRACTION

Parameter	**Data**
pK_a	2.98 - 5.28
CASRN and Test Material	Not Reported; phthalic acid
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	not reported
System	not reported
pH	not reported
Results Details Method	not reported
Standard Deviation Results	Not Reported
Results Details	pKa1 = 2.98; pKa2 = 5.28

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's similarity to values included in distiller.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: cites: W. R. Maxwell and J. R. Partington, The Dissociation Constants of Some Polybasic Acids, Trans. Faraday Soc., 1937, 33, 670. No HERO IDE. A. Braude and F. C. Nachod, Determination of Organic Structures by Physical Methods, New York, Academic Press, 1955. No HERO ID

Study Citation:	Tummanapelli, A. K., Vasudevan, S. (2015). Estimating successive pKa values of polyprotic acids from ab initio molecular dynamics using metadynamics: the dissociation of phthalic acid and its isomers. Physical Chemistry Chemical Physics 17(9):6383-6388.
OECD Harmonized Template:	pKa
HERO ID:	4278044

EXTRACTION

Parameter	**Data**
pK_a	2.91 - 5.09
CASRN and Test Material	Not Reported; phthalic acid
Confidentiality, Type, and Guideline	no; calculation; simulation methodology
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	300 K
System	ab initio molecular dynamics simulation
pH	not applicable
Results Details Method	Not Reported
Standard Deviation Results	gradient corrected exchange correlational DFT-HCTH/120 functional was used
Results Details	pKa1 = 2.91; pKa2 = 5.09

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Calculated data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Myhre, L., C.E., Nielsen, C. J. (2004). Optical properties in the UV and visible spectral region of organic acids relevant to tropospheric aerosols. Atmospheric Chemistry and Physics 4(7):1759-1769.
OECD Harmonized Template:	Refractive Index
HERO ID:	3339378

EXTRACTION

Parameter	**Data**
Refractive Index	1.3322 - 1.3326
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	Water; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	293±0.5 K
System	Thermostated Abbe Standard 60 refractometer, 15798 /cm, He-Ne laser
Standard Deviation Results	Not Reported
Results Details	Measured at 632.8 nm, 0.07 and 0.11% wt solution. Average of 4 replicates.
Results Details Methods	Not Reported
Parameter	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytic methods.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Myhre, L., C.E., Nielsen, C. J. (2004). Optical properties in the UV and visible spectral region of organic acids relevant to tropospheric aerosols. Atmospheric Chemistry and Physics 4(7):1759-1769.
OECD Harmonized Template:	Refractive Index
HERO ID:	3339378

EXTRACTION

Parameter	**Data**
Refractive Index	1.3322 - 1.3326
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	293 K
System	The wavelength dependent refractive index, n(), in the region from 275–1100 nm was determined from the absorption index and using the measured index of refraction at 632.8 nm as anchor point.
Standard Deviation Results	0.15%
Results Details	concentration 0.07 wt% with pH 2.75 and 0.11 wt% with pH 2.67 at 293K
Results Details Methods	Not Reported
Parameter	Not Reported

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	RSC, (2020). ChemSpider: phthalic acid.
OECD Harmonized Template:	Refractive Index
HERO ID:	7274515

EXTRACTION

Parameter	**Data**
Refractive Index	1.756
CASRN and Test Material	88-99-3; Phthalic acid
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not reported
System	Not Reported
Standard Deviation Results	Not reported
Results Details	Not reported
Results Details Methods	Not Reported
Parameter	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: SynQuest

List of Abbreviations and Acronyms for Data Quality Evaluation and Extraction Tables

Term	Definition
ASTM	American Society for Testing and Materials
ATSDR	Agency for Toxic Substances and Disease Registry
atm	Atmospheres
atm · m^3/mol	Atmospheres - cubic meters per mole
C	Celsius
CASRN	Chemical Abstract Service registry number
cP	Centipoise
CRC	CRC Handbook of Chemistry and Physics
DOE	U.S. Department of Energy
ECB	European Chemicals Bureau
EPA	Environmental Protection Agency
F	Fahrenheit
GC	Gas Chromatography
g/cm^3	Grams per cubic centimeter
GLP	Good Laboratory Practice
HLC	Henry's Law Constant
HPV	High Production Volume
HSDB	Hazard Substance Data Bank
ILO	International Labour Organization
IPCS	International Programme on Chemical Safety
IUCLID	International Uniform Chemical Information Database
K	Kelvin
Koa	Octanol-Air partition coefficient
Kow	Octanol-Water partition coefficient
mg/L	Milligrams per Liter
mol	Mole
mmHg	Millimeters of Mercury
MS	Mass Spectrometry
N/A	Not Applicable
NICNAS	National Industrial Chemicals Notification and Assessment Scheme
NLM	National Library of Medicine
NR	Not Reported
OECD	Organisation for Economic Co-operation and Development
Pa (hPa)	Pascals (hectopascals; 1 hPa = 100 Pa)
pH	Negative base 10 Log of Hydrogen Ion (H+) Concentration in Aqueous Solution
pKa	Negative base 10 Log of Acid Dissociation Constant (Ka)
RIVM	National Institute for Public Health and the Environment (Dutch: Rijksinstituut voor Volksgezondheid en Milieu)

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Term	Definition
RSC	Royal Society of Chemistry
RT	Retention Time
SIDs	Screening Information Dataset
VP	Vapor Pressure
US or USA	United States of America
UV (UV-Vis)	Ultra Violet (UV-Visible)
WHO	World Health Organization