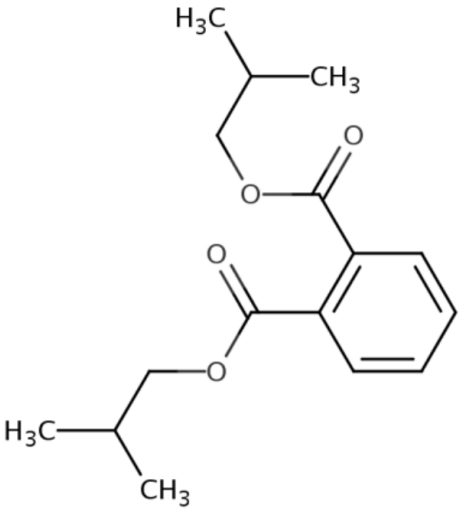
United States
Environmental Protection Agency

July 2025
Office of Chemical Safety and
Pollution Prevention

Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties for Di-isobutyl Phthalate (DIBP) (1,2-Benzenedicarboxylic acid, 1,2-bis(2-methylpropyl) ester)

Systematic Review Support Document for the Draft Risk Evaluation

CASRN: 84-69-5



July 2025

This supplemental file contains information regarding the data extraction and evaluation results for data sources that were considered for the *Draft Risk Evaluation for Diisobutyl Phthalate (DIBP)* 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 Diisobutyl Phthalate (DIBP)*. 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.

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Study Citation:	CPSC, (2015). Exposure assessment: Composition, production, and use of phthalates.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5155508

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-69-5; di-isobutyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; liquid; NR
Results Value	Mostly odorless
Results Details	Not Reported

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	The information is related to 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 peer-review.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — High

* Related References: CPSC (U.S. Consumer Product Safety Commission). 2010. Review of Exposure Data and Assessments for Selected Dialkyl Ortho-Phthalates. CPSC-D-06-0006. Consumer Product Safety Commission, Bethesda, MD.

Study Citation:	ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes.
OECD Harmonized Template:	Physical Form or State
HERO ID:	7325405

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-69-5; Di-isobutyl phthalate
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; liquid; NR
Results Value	Colourless liquid
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)	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: Source cited: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Study Citation:	Haz-Map, (2021). Hazardous agents: Diisobutyl phthalate.
OECD Harmonized Template:	Physical Form or State
HERO ID:	8486308

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-69-5; 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 Value	Colorless viscous liquid
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	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

* Related References: Citing ICSC

Study Citation:	U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).
OECD Harmonized Template:	Physical Form or State
HERO ID:	5155528

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-69-5; Not Reported
Confidentiality, Type, and Guideline	None; 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 Value	Colorless, clear, mostly odorless, viscous liquid
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	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: Cites secondary sources:NICNAS (National Industrial Chemicals Notification and Assessment Scheme). (2008) Diisobutyl phthalate. Existing chemical hazard assessment report. Australian Government. Available online at: http://www.nicnas.gov.au/Publications/CAR/Other/DiBPP%20hazard%20assessment.pdf(accessed October 13, 2010). HEROID 5155528. ECHA (European Chemicals Agency). (2009) Annex IV Dossier, proposal for identification of a substance as SVHC/CMR (substances of very high concern/carcinogenic, mutagenic, or toxic to reproduction). http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdfHEROID unknown Not previously extracted. HEROID in distiller.

Study Citation:	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926117

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	liquid
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: Lewis, R.J. Sr. 2007. Hawley's Condensed Chemical Dictionary. 15th Edition. John Wiley & Sons, Inc. New York, NY. P. 434.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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: Value reported by multiple primary sources in REAXYS.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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 diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	red

EVALUATION

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:	EC/HC, (2015). State of the science report: Phthalate substance grouping: Medium-chain phthalate esters: Chemical Abstracts Service Registry Numbers: 84-61-7; 84-64-0; 84-69-5; 523-31-9; 5334-09-8;16883-83-3; 27215-22-1; 27987-25-3; 68515-40-2; 71888-89-6.
OECD Harmonized Template:	Melting Point
HERO ID:	3688160

EXTRACTION

Parameter	**Data**
Melting Point	-52 °C
CASRN and Test Material	84-69-5; diisobutyl phthalate
Confidentiality, Type, and Guideline	no; experimental; not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; liquid; 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	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: cites: [ECHA] European Chemicals Agency. c2007–2014b. Registered substances database. Search for CAS RN 84-69-5 [DIBP]. Helsinki (FI): ECHA. [cited 2014 Sept] Available from: http://echa.europa.eu/information-on-chemicals/registered-substances;jsessionid=ADE5DCC9E32E9AC042ACD435168FEB84.live1?p_auth=UvS8Lp1d&p_p_id=registeredsubstances_WAR_regsubsportlet&p_p_lifecycle=1&p_p_state=normal&p_p_mode=vi 1&p_p_col_pos=1&p_p_col_count=6&_registeredsubstances_WAR_regsubsportlet_javax.portlet.action=registeredSubstancesAction

Study Citation:	ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates.
OECD Harmonized Template:	Melting Point
HERO ID:	3661424

EXTRACTION

Parameter	**Data**
Melting Point	-37 °C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; liquid; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	1,013 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	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 Low

* Related References: referenced to HEROID: 680273: Annex XV dossier, 2009. Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009.

Study Citation:	ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes.
OECD Harmonized Template:	Melting Point
HERO ID:	7325405

EXTRACTION

Parameter	**Data**
Melting Point	-37 °C
CASRN and Test Material	84-69-5; Di-isobutyl phthalate
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; liquid; NR
Results Details Methods	at 1013 hPa
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: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Melting Point
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
Melting Point	-58 °C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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.
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: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb. 4; (1997); p. 667 - 749

Study Citation:	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.
OECD Harmonized Template:	Melting Point
HERO ID:	5926117

EXTRACTION

Parameter	**Data**
Melting Point	-64 °C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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: Clayton, G.D., Clayton, F.E. (Eds.) 1981. Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd Ed. New York: John Wiley Sons. P. 2345.

Study Citation:	RSC, (2019). ChemSpider: Diisobutyl phthalate.
OECD Harmonized Template:	Melting Point
HERO ID:	5926262

EXTRACTION

Parameter	**Data**
Melting Point	-64 °C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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: Biosynth

Study Citation:	U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).
OECD Harmonized Template:	Melting Point
HERO ID:	5155528

EXTRACTION

Parameter	**Data**
Melting Point	-50 - °C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	No; not specified; NR
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.
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: Cites secondary sources:European Commission. (2000) Substance ID: 84-69-5. Diisobutyl phthalate. IUCLID Dataset.European Commission. European Chemicals Bureau. Available online at http://ecb.jrc.ec.europa.eu/iuclid-datasheet/84695.pdf (accessed April 13, 2011).HEROID 680279

Study Citation:	U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).
OECD Harmonized Template:	Melting Point
HERO ID:	5155528

EXTRACTION

Parameter	**Data**
Melting Point	-42 - °C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	No; not specified; NR
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.
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: Cites secondary sources:European Commission. (2000) Substance ID: 84-69-5. Diisobutyl phthalate. IUCLID Dataset.European Commission. European Chemicals Bureau. Available online at http://ecb.jrc.ec.europa.eu/iuclid-datasheet/84695.pdf (accessed April 13, 2011).HEROID 680279

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Diisobutyl phthalate. 84-69-5..
OECD Harmonized Template:	Melting Point
HERO ID:	5926150

EXTRACTION

Parameter	**Data**
Melting Point	-64 °C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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 Diisobutyl phthalate. 84-69-5..
OECD Harmonized Template:	Melting Point
HERO ID:	5926150

EXTRACTION

Parameter	**Data**
Melting Point	-64 °C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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 Diisobutyl phthalate. 84-69-5..
OECD Harmonized Template:	Melting Point
HERO ID:	5926150

EXTRACTION

Parameter	**Data**
Melting Point	-64 °C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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:	Wang, L. M., Richert, R. (2007). Glass transition dynamics and boiling temperatures of molecular liquids and their isomers. Journal of Physical Chemistry B 111(12):3201-3207.
OECD Harmonized Template:	Melting Point
HERO ID:	680451

EXTRACTION

Parameter	**Data**
Melting Point	191.1 K
CASRN and Test Material	84-69-5; Di-iso-butylphthalate
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; Stable in temperature ranges to the glass transition temperature
Radiolabel, Source, State, and Purity	NR; Aldrich; NR; 99%
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Value is a glass transition 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's 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	The analytical method is non-standard but is expected to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	Data are 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:	CPSC, (2015). Exposure assessment: Composition, production, and use of phthalates.
OECD Harmonized Template:	Boiling Point
HERO ID:	5155508

EXTRACTION

Parameter	**Data**
Boiling Point	159 C
CASRN and Test Material	84-69-5; di-isobutyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; liquid; NR
Standard Deviation Results	Not Reported
Results Details	at 4 mm Hg

EVALUATION

Domain	Metric		Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	The data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with other physical 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	The data are from a source that is known but is missing peer-review.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: HSDB (Hazardous Substances Data Bank). 2015. Hazardous Substances Data Bank online database, Toxnet Toxicology Data Network. U.S. National Library of Medicine. Available at: http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB

Study Citation:	ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes.
OECD Harmonized Template:	Boiling Point
HERO ID:	7325405

EXTRACTION

Parameter	**Data**
Boiling Point	320 C
CASRN and Test Material	84-69-5; Di-isobutyl phthalate
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; liquid; NR
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	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: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
Boiling Point	295 - 327 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	5 values were reported in Reaxys; 4 values were reported in the range of 295 to 327 C at unreported pressures; 1 value was reported at non-standard 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'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:	NIST, (2022). NIST Chemistry WebBook. 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester (84-69-5). Standard Reference Database No. 69.
OECD Harmonized Template:	Boiling Point
HERO ID:	10225182

EXTRACTION

Parameter	**Data**
Boiling Point	593 - K
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	No; Not specified; NR
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	Uncertainty assigned by TRC = 4. 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	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	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 Low

* Related References: Citing Haertel, G.H., Low-volatility polar organic solvents for sulfur dioxide, hydrogen sulfide, and carbonyl sulfide., J. Chem. Eng. Data, 1985, 30, 57. HERO ID 2797985.

Study Citation:	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926117

EXTRACTION

Parameter	**Data**
Boiling Point	296.5 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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.) 2010. CRC Handbook of Chemistry and Physics. 91st Edition. Boca Raton, FL: CRC Press Inc. p. 3-184.

Study Citation:	RSC, (2019). ChemSpider: Diisobutyl phthalate.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926262

EXTRACTION

Parameter	**Data**
Boiling Point	295.3 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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: Biosynth

Study Citation:	RSC, (2019). ChemSpider: Diisobutyl phthalate.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926262

EXTRACTION

Parameter	**Data**
Boiling Point	327 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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). Diisobutyl phthalate. :3-20.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926366

EXTRACTION

Parameter	**Data**
Boiling Point	296.5 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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:	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	296.5
CASRN and Test Material	Not Reported; Di-isobutyl phthalate
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:	U.S. EPA, (2019). Chemistry Dashboard Information for Diisobutyl phthalate. 84-69-5..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926150

EXTRACTION

Parameter	**Data**
Boiling Point	296 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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 Diisobutyl phthalate. 84-69-5..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926150

EXTRACTION

Parameter	**Data**
Boiling Point	327 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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 Diisobutyl phthalate. 84-69-5..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926150

EXTRACTION

Parameter	**Data**
Boiling Point	327 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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:	Wang, L. M., Richert, R. (2007). Glass transition dynamics and boiling temperatures of molecular liquids and their isomers. Journal of Physical Chemistry B 111(12):3201-3207.
OECD Harmonized Template:	Boiling Point
HERO ID:	680451

EXTRACTION

Parameter	**Data**
Boiling Point	552 K
CASRN and Test Material	84-69-5; Di-iso-butylphthalate
Confidentiality, Type, and Guideline	None; Calculation; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; Stable in temperature ranges to the glass transition temperature
Radiolabel, Source, State, and Purity	NR; Aldrich; NR; 99%
Standard Deviation Results	Not Reported
Results Details	Boiling point calculated from experimentally derived relationship to measured glass transition temperature Tb = 132 + 2.2Tg (where Tg > 45 K). Tg = 191.1 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's 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	The analytical method is non-standard but is expected to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	Data are from a primary peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation:	Cao, X. L. (2010). Phthalate esters in foods: Sources, occurrence, and analytical methods. Comprehensive Reviews in Food Science and Food Safety 9(1):21-43.
OECD Harmonized Template:	Density
HERO ID:	1322045

EXTRACTION

Parameter	**Data**
Density	1.039 g/mL
CASRN and Test Material	84-69-5; di-iso-butyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Density Type	Not Reported
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 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 toward a particular 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 secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a peer-reviewed secondary source without inclusion of references to the original sources.
	Metric 6:	Models	N/A	The metric is not applicable to the study type.

Overall Quality Determination Medium

Study Citation:	EC/HC, (2015). State of the science report: Phthalate substance grouping: Medium-chain phthalate esters: Chemical Abstracts Service Registry Numbers: 84-61-7; 84-64-0; 84-69-5; 523-31-9; 5334-09-8;16883-83-3; 27215-22-1; 27987-25-3; 68515-40-2; 71888-89-6.
OECD Harmonized Template:	Density
HERO ID:	3688160

EXTRACTION

Parameter	**Data**
Density	1049 kg/m3
CASRN and Test Material	84-69-5; diisobutyl phthalate
Confidentiality, Type, and Guideline	no; experimental; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; liquid; NR
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	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: cites: Haynes WM, Lide DR. 2010. CRC Handbook of Chemistry and Physics. 91st edition.2010-2011. Boca Raton (FL): CRC Press, Taylor & Francis Group.

Study Citation:	U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).
OECD Harmonized Template:	Density
HERO ID:	5155528

EXTRACTION

Parameter	**Data**
Density	1.038 - g/cm3
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	None; not specified; NR
Solvent, Reactivity, Storage, and Stability	NR; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	density
System	NR
Temperature	NR
Standard Deviation Results	Not Reported
Results Details	Reported as 1038 kg/m^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	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: Cites secondary sources:NICNAS (National Industrial Chemicals Notification and Assessment Scheme). (2008)Diisobutyl phthalate. Existing chemical hazard assessment report. Australian Government.Available online at http://www.nicnas.gov.au/Publications/CAR/Other/DiBPP%20hazard%20assessment.pdf(accessed October 13, 2010). HEROID 2316625 Not previously extracted, not in distiller.

Study Citation:	U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).
OECD Harmonized Template:	Density
HERO ID:	5155528

EXTRACTION

Parameter	**Data**
Density	1.037 - 1.049 g/cm3
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	None; not specified; NR
Solvent, Reactivity, Storage, and Stability	NR; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	density
System	NR
Temperature	20 deg 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	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: Cites secondary sources:European Commission. (2000) Substance ID: 84-69-5. Diisobutyl phthalate. IUCLID Dataset.European Commission. European Chemicals Bureau. Available online at http://ecb.jrc.ec.europa.eu/iuclid-datasheet/84695.pdf (accessed April 13, 2011).HEROID 680279Not previously extracted, not in distiller.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Density
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
Density	1.036 - 1.0412 g/cm3
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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; 3 values were reported in Reaxys; 2 values were reported in the range of 1.036 to 1.0412 at 20°C; 1 value (1.049) was reported at a non-standard 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	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: Data range determined from multiple primary sources in REAXYS.

Study Citation:	RSC, (2019). ChemSpider: Diisobutyl phthalate.
OECD Harmonized Template:	Density
HERO ID:	5926262

EXTRACTION

Parameter	**Data**
Density	1.039 g/cm3
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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. (2018). Diisobutyl phthalate. :3-20.
OECD Harmonized Template:	Density
HERO ID:	5926366

EXTRACTION

Parameter	**Data**
Density	1.0490 g/cm3
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	15°C
Standard Deviation Results	Not Reported
Results Details	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	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 Compound Summary for CID 6782 Diisobutyl phthalate.
OECD Harmonized Template:	Density
HERO ID:	6629592

EXTRACTION

Parameter	**Data**
Density	9.59
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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
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 reported for the target 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 secondary database with a reference to another database.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

* Related References: CAMEO Chemicals: 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 Compound Summary for CID 6782 Diisobutyl phthalate.
OECD Harmonized Template:	Density
HERO ID:	6629592

EXTRACTION

Parameter	**Data**
Density	9.6
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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
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 reported for the target 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 secondary database with a reference to a 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: ILO International Chemical Safety Cards (ICSC)

Study Citation:	Cao, X. L. (2010). Phthalate esters in foods: Sources, occurrence, and analytical methods. Comprehensive Reviews in Food Science and Food Safety 9(1):21-43.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	1322045

EXTRACTION

Parameter	**Data**
Vapor Pressure	4.73x10-3 Pa
CASRN and Test Material	84-69-5; di-iso-butyl phthalate
Confidentiality, Type, and Guideline	no; not specified; 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	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 (e.g., presence of certain functional groups) or other 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 toward a particular 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 secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a peer-reviewed secondary source without inclusion of 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

Study Citation:	EC/HC, (2015). State of the science report: Phthalate substance grouping: Medium-chain phthalate esters: Chemical Abstracts Service Registry Numbers: 84-61-7; 84-64-0; 84-69-5; 523-31-9; 5334-09-8;16883-83-3; 27215-22-1; 27987-25-3; 68515-40-2; 71888-89-6.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	3688160

EXTRACTION

Parameter	**Data**
Vapor Pressure	6.3×10-3 Pa
CASRN and Test Material	84-69-5; diisobutyl phthalate
Confidentiality, Type, and Guideline	no; experimental; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; liquid; 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	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

* Related References: cites: Daubert TE, Danner RP. 1989. Physical and thermodynamic properties of purechemicals data compilation. Washington (DC): Taylor and Francis [cited in HSDB 2010].

Study Citation:	ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	7325405

EXTRACTION

Parameter	**Data**
Vapor Pressure	0.01 Pa
CASRN and Test Material	84-69-5; Di-isobutyl phthalate
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; liquid; NR
Temperature	20°C
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	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: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
Vapor Pressure	2E-6 - 5.8E-4 mm Hg
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	2 data points were reported in Reaxys; 2 values were reported at 2E-6 to 5.8E-4 torr 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'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: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb. 4; (1997); p. 667 - 749

Study Citation:	Haz-Map, (2021). Hazardous agents: Diisobutyl phthalate.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	8486308

EXTRACTION

Parameter	**Data**
Vapor Pressure	= 0.00665 mm Hg
CASRN and Test Material	84-69-5; Di-isobutyl phthalate
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
Temperature	not specified
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	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:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	3475635

EXTRACTION

Parameter	**Data**
Vapor Pressure	0.010 Pa
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.
Temperature	298.15 K
System	System uses dynamic gas saturation method between 313.15 and 423.15K, using the Clausius-Clapeyron equation to fit to standard temperature (298.15 K).
Standard Deviation Results	NA
Results Details	Value is extrapolated from vapor pressures measured between 313.15 K and 423.15 K.

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 (e.g., presence of certain functional groups).
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 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:	Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	807140

EXTRACTION

Parameter	**Data**
Vapor Pressure	6.20X10-3 Pa
CASRN and Test Material	84-74-2; diisobutyl phthalate
Confidentiality, Type, and Guideline	none; QSAR; Quantitative Structure-Property relationship model for estimation of solubility in air
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: DIBP
Temperature	Not Reported
System	Predictive model developed using gas law: S(A) = P(liquid substance)/RT where R= gas constant (8.314 Pa m-3 mol-1 K-1) and T = absolute temperature (298K); Log S(A) = -0.2324 - 0.3215 (Lu)
Standard Deviation Results	Not Reported
Results Details	Log S(A): n = 15; correlation coefficient (R) = 0.9461; standard error (SE) = 0.27; leave-one-out cross validation correlation coefficient (Rsv) = 0.9218; corresponding standard errors (scv) = 0.34

EVALUATION

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	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 AND the model performance was known and r2 $>$ 0.7, q2 $>$ 0.5, and SE $<$ 0.3 (ECHA, 2016).

Overall Quality Determination High

Study Citation:	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926117

EXTRACTION

Parameter	**Data**
Vapor Pressure	4.76E-5 mm Hg
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	from experimentally derived coefficients

EVALUATION

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

Study Citation:	Cao, X. L. (2010). Phthalate esters in foods: Sources, occurrence, and analytical methods. Comprehensive Reviews in Food Science and Food Safety 9(1):21-43.
OECD Harmonized Template:	logKow
HERO ID:	1322045

EXTRACTION

Parameter	**Data**
log k_{ow}	4.27
CASRN and Test Material	84-69-5; di-iso-butyl phthalate
Confidentiality, Type, and Guideline	no; not specified; 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	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 (e.g., presence of certain functional groups) or other 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 toward a particular 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 secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a peer-reviewed secondary source without inclusion of 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

Study Citation:	ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes.
OECD Harmonized Template:	logKow
HERO ID:	7325405

EXTRACTION

Parameter	**Data**
log k_{ow}	4.11
CASRN and Test Material	84-69-5; Di-isobutyl phthalate
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; liquid; NR
Temperature	not specified
System	not specified
pH	not specified
Results Details Method	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	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: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	logKow
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
log k_{ow}	4.31 - 4.86
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	@ 25 C; 5 values were reported in Reaxys; 3 values were reported at 4.31 to 4.86 at 25 C; 2 values were reported at 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	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:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	logKow
HERO ID:	3475635

EXTRACTION

Parameter	**Data**
log k_{ow}	4.34
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.
Temperature	298.15 K
System	Shake-flask method with n-octanol and purified water, quantified by HPLC-UV.
pH	Not reported
Results Details Method	n-Octanol pre-saturated water with the test substance is poured into a test vessel and stirred with a magnetic stirring bar. 100 g of the aqueous phase is analyzed through C-18 cartridges and eluted with methanol. The concentration of the solute is then quantified by HPLC-UV.
Standard Deviation Results	0.082
Results Details	Value the average of 3 replicates at atmospheric 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.
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. Methodology reported in J. Saab, G. Basil, R. About Niccol, J. Stephan, I. Mokbel, J. Jose, Chemosphere 82 (2011) 929-934.
	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 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:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	logKow
HERO ID:	3475635

EVALUATION

Domain	Metric	Rating	Comments

Study Citation:	Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173.
OECD Harmonized Template:	logKow
HERO ID:	807140

EXTRACTION

Parameter	Data
log k_{ow}	4.08
CASRN and Test Material	84-69-5; diisobutyl phthalate
Confidentiality, Type, and Guideline	none; QSAR; Quantitative Structure-Property relationship model for estimation of log Kow
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: DIBP
Temperature	not applicable
System	QSPR model using the Lu index, which is based on the shortest distance matrix.
pH	not applicable
Results Details Method	Predictive model developed using Lu index: Log Kow = -4.7875 + 0.5315 (Lu)
Standard Deviation Results	Not Reported
Results Details	n = 15; correlation coefficient (R) = 0.9836; standard error (SE) = 0.40; leave-one-out cross validation correlation coefficient (Rsv) = 0.9784; corresponding standarderrors (scv) = 0.47

EVALUATION

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	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	Uninformative	The QSPR model failed the standard error threshold of <0.3 and is therefore rated unacceptable.

Overall Quality Determination — Medium

Study Citation:	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.
OECD Harmonized Template:	logKow
HERO ID:	5926117

EXTRACTION

Parameter	**Data**
log k_{ow}	4.11
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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 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: Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society, 1995, p. 144

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Diisobutyl phthalate. 84-69-5..
OECD Harmonized Template:	logKow
HERO ID:	5926150

EXTRACTION

Parameter	**Data**
log k_{ow}	4.11
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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:	Aktiengesellschaft,, BASF (2001). [Redacted] Physico-chemical properties of "Palatinol IC".
OECD Harmonized Template:	Water Solubility
HERO ID:	11182936

EXTRACTION

Parameter	**Data**
Water Solubility	11.5 - mg/L
CASRN and Test Material	Not Reported; diisobutyl phthalate
Confidentiality, Type, and Guideline	None; experimental; Ammex Commission Directive 92/69/EEC, A6, flask method
Solvent, Reactivity, Storage, and Stability	NR; NR; ambient; NR
Radiolabel, Source, State, and Purity	NA; Palatinol IC from Weichmacherfabrik (plasticizer factory), CPW/WA-M800; NR; not known Notes: Batch B4118 Partie:23/01
Temperature	25ºC ±2ºC
System	Stirred at 30ºC for 24, 48 and 72 hours and conditioned at 25ºC for >1 day. The water phase was separated and extracted with chloroform 3 times. The chloroform was dried and evaporated.
pH	7
Results Details Method	GC analysis
Standard Deviation Results	0.3 mg/L
Results Details	11.5 mg/L (mean value of 3 samples 11.6, 11.2 and 11.7 mg/L at pH 6.8, 6.7 and 7.0)

EVALUATION

Domain		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:	Cao, X. L. (2010). Phthalate esters in foods: Sources, occurrence, and analytical methods. Comprehensive Reviews in Food Science and Food Safety 9(1):21-43.
OECD Harmonized Template:	Water Solubility
HERO ID:	1322045

EXTRACTION

Parameter	**Data**
Water Solubility	9.9 mg/L
CASRN and Test Material	84-69-5; di-iso-butyl phthalate
Confidentiality, Type, and Guideline	no; not specified; 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	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 (e.g., presence of certain functional groups) or other 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 toward a particular 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 secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a peer-reviewed secondary source without inclusion of 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

Study Citation:	CPSC, (2015). Exposure assessment: Composition, production, and use of phthalates.
OECD Harmonized Template:	Water Solubility
HERO ID:	5155508

EXTRACTION

Parameter	**Data**
Water Solubility	1.1x10-3 g/L
CASRN and Test Material	84-69-5; di-isobutyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; liquid; 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	The data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with other 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	The data are from a publicly available source without peer-review.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination — Medium

* Related References: CPSC (U.S. Consumer Product Safety Commission). 2010. Review of Exposure Data and Assessments for Selected Dialkyl Ortho-Phthalates. CPSC-D-06-0006. Consumer Product Safety Commission, Bethesda, MD.

Study Citation:	EC/HC, (2017). Draft screening assessment: Phthalate substance grouping.
OECD Harmonized Template:	Water Solubility
HERO ID:	5353181

EXTRACTION

Parameter	**Data**
Water Solubility	20.3 mg/L
CASRN and Test Material	84-69-5; diisobutyl phthalate
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 specified
System	not specified
pH	not specified
Results Details Method	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: Haynes and Lide 2010

Study Citation:	ECETOC, (1985). An assessment of the occurrence and effects of dialkyl ortho-phthalates in the environment.
OECD Harmonized Template:	Water Solubility
HERO ID:	679967

EXTRACTION

Parameter	**Data**
Water Solubility	1E5 ug/L
CASRN and Test Material	Not Reported; Diisobutyl phthalate
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 deg 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 substance structural features.
Domain 2: Test Reliability				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Low	The present authors believe that value are wrong in the light of the other figures quoted.
	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 — Low

* Related References: Citing Fishbein and Albro (1972), HERO ID 1313257.

Study Citation:	ECETOC, (1985). An assessment of the occurrence and effects of dialkyl ortho-phthalates in the environment.
OECD Harmonized Template:	Water Solubility
HERO ID:	679967

EXTRACTION

Parameter	**Data**
Water Solubility	2E4 ug/L
CASRN and Test Material	Not Reported; Diisobutyl phthalate
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 deg 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 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	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: Citing Leyder and Boulanger (1983) HERO ID 679764.

Study Citation:	ECETOC, (1985). An assessment of the occurrence and effects of dialkyl ortho-phthalates in the environment.
OECD Harmonized Template:	Water Solubility
HERO ID:	679967

EXTRACTION

Parameter	**Data**
Water Solubility	6E3 ug/L
CASRN and Test Material	Not Reported; Diisobutyl phthalate
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	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	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: Citing Hollifield, H.C. (1974). Rapid nephetometric estimate of water solubility ofhighly insoluble organic chemicals of environmental interest. Bull. Envir.Contam. Toxicol., 23, 579. no HERO ID.

Study Citation:	ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes.
OECD Harmonized Template:	Water Solubility
HERO ID:	7325405

EXTRACTION

Parameter	**Data**
Water Solubility	20 mg/L
CASRN and Test Material	84-69-5; Di-isobutyl phthalate
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; liquid; NR
Temperature	20°C
System	not specified
pH	not specified
Results Details Method	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	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: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Water Solubility
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
Water Solubility	5.1 - 9.6 mg/L
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	Reported as 0.0051 to 0.0096 g/L at 25 C
Standard Deviation Results	Not Reported
Results Details	2 data points were reported in Reaxys; 2 values were reported as 0.0051 to 0.0096 g/L at standard 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'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: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb. 4; (1997); p. 667 - 749

Study Citation:	Hollifield, H. C. (1979). Rapid nephelometric estimate of water solubility of highly insoluble organic chemicals of environmental interest. Bulletin of Environmental Contamination and Toxicology 23(4-5):579-586.
OECD Harmonized Template:	Water Solubility
HERO ID:	7401366

EXTRACTION

Parameter	**Data**
Water Solubility	6.2 mg/L
CASRN and Test Material	Not Reported; diisobutyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	0.5% or less stock in ethanol or acetone. Adjusted with same solvent until 0.5 -1.5 mL standard produced turbid suspension in 40 mL water.; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; Liquid; NR
Temperature	24±2°C
System	Spectrophotofluorometer with a photomultiplier photometer, potted photomultiplier tube, and 150 W xenon arc lamp; test substance analyzed in standard 1-cm path length quartz fluorescence cuvette.
pH	Not reported
Results Details Method	Study performed at constant slit width, 3,2,2,3,5 slit arrangement. Excitation and emission monochromators set to 600 nm.
Standard Deviation Results	Not Reported
Results Details	40 mL water, 1 mL gum tragacanth solution (stock 0.10 g/L in water) used to prevent suspensions, and test substance added by syringe at 0.1 mL/min were stirred by magnetic stirrer until first signs of turbidity. This was repeated with 0.1 mL increasing quantities of test substance to create 6-8 standards. Turbid solutions allowed to rest for 15 min, resuspended by stirring, and nephelometric measurements were recorded. Calibration curve extrapolated to blank prepared without test substance to determine solubility.

EVALUATION

Domain		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	The analytical method is non-standard 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

* Related References: Citing METCALF, R.L. and P.Y. LU: "Environmental Distribution and Metabolic Fate of Key Industrial Pollutants and Pesticides in a Model Ecosystem," Research Report No. 69, University of Illinois Water Resources Center, 72 (1973).

Study Citation:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	Water Solubility
HERO ID:	3475635

EXTRACTION

Parameter	**Data**
Water Solubility	7.080E-7
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.
Temperature	298.15 K
System	Water solubility measured using a dynamic saturation apparatus with quantification via HPLC-UV. Methanol was used as the solvent for elution.
pH	Not reported
Results Details Method	Temperature measurement accuracy was ±0.02 K.
Standard Deviation Results	2.54E-6
Results Details	Value reported as mole fraction, where mole fraction = n solute / (n water + n solute). The value could not be converted to standard units as the volume of water used was not reported in this paper. Value initially reported as 7.080E7 but based on later references to solubilities of "10^-7", this is believed to be a typo. Average of three replicates measured at atmospheric 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	Medium	Data cannot be converted to standard units and therefore appropriateness cannot be verified, but is likely to be appropriate based on the data's inclusion in a peer-reviewed article.
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.
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:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	Water Solubility
HERO ID:	3475635

EVALUATION

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

Study Citation:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	Water Solubility
HERO ID:	3475635

EXTRACTION

Parameter	**Data**
Water Solubility	7.051E-7
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.
Temperature	303.15 K
System	Water solubility measured using a dynamic saturation apparatus with quantification via HPLC-UV. Methanol was used as the solvent for elution.
pH	Not reported
Results Details Method	Temperature measurement accuracy was ±0.02 K.
Standard Deviation Results	1.68E-1
Results Details	Value reported as mole fraction, where mole fraction = n solute / (n water + n solute). The value could not be converted to standard units as the volume of water used was not reported in this paper. Value initially reported as 7.051E7 but based on later references to solubilities of "10^-7", this is believed to be a typo. Average of three replicates measured at atmospheric 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	Medium	Data cannot be converted to standard units and therefore appropriateness cannot be verified, but is likely to be appropriate based on the data's inclusion in a peer-reviewed article.
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.
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

Study Citation:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	Water Solubility
HERO ID:	3475635

EXTRACTION

Parameter	**Data**
Water Solubility	8.072E-7
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.
Temperature	308.15 K
System	Water solubility measured using a dynamic saturation apparatus with quantification via HPLC-UV. Methanol was used as the solvent for elution.
pH	Not reported
Results Details Method	Temperature measurement accuracy was ±0.02 K.
Standard Deviation Results	2.01E-1
Results Details	Value reported as mole fraction, where mole fraction = n solute / (n water + n solute). The value could not be converted to standard units as the volume of water used was not reported in this paper. Value initially reported as 8.072E7 but based on later references to solubilities of "10^-7", this is believed to be a typo. Average of three replicates measured at atmospheric 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	Medium	Data cannot be converted to standard units and therefore appropriateness cannot be verified, but is likely to be appropriate based on the data's inclusion in a peer-reviewed article.
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.
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

Study Citation:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	Water Solubility
HERO ID:	3475635

EXTRACTION

Parameter	**Data**
Water Solubility	8.590E-7
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.
Temperature	313.15 K
System	Water solubility measured using a dynamic saturation apparatus with quantification via HPLC-UV. Methanol was used as the solvent for elution.
pH	Not reported
Results Details Method	Temperature measurement accuracy was ±0.02 K.
Standard Deviation Results	4.20E-5
Results Details	Value reported as mole fraction, where mole fraction = n solute / (n water + n solute). The value could not be converted to standard units as the volume of water used was not reported in this paper. Value initially reported as 8.590E7 but based on later references to solubilities of "10^-7", this is believed to be a typo. Average of three replicates measured at atmospheric 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	Medium	Data cannot be converted to standard units and therefore appropriateness cannot be verified, but is likely to be appropriate based on the data's inclusion in a peer-reviewed article.
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.
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

Study Citation:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	Water Solubility
HERO ID:	3475635

EXTRACTION

Parameter	**Data**
Water Solubility	11.254E-7
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.
Temperature	323.15 K
System	Water solubility measured using a dynamic saturation apparatus with quantification via HPLC-UV. Methanol was used as the solvent for elution.
pH	Not reported
Results Details Method	Temperature measurement accuracy was ±0.02 K.
Standard Deviation Results	1.57E-6
Results Details	Value reported as mole fraction, where mole fraction = n solute / (n water + n solute). The value could not be converted to standard units as the volume of water used was not reported in this paper. Value initially reported as 11.254E7 but based on later references to solubilities of "10^-7", this is believed to be a typo. Average of three replicates measured at atmospheric 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	Medium	Data cannot be converted to standard units and therefore appropriateness cannot be verified, but is likely to be appropriate based on the data's inclusion in a peer-reviewed article.
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.
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

Study Citation:	Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173.
OECD Harmonized Template:	Water Solubility
HERO ID:	807140

EXTRACTION

Parameter	**Data**
Water Solubility	13.8 mg/L
CASRN and Test Material	84-69-5; diisobutyl phthalate
Confidentiality, Type, and Guideline	none; QSAR; Quantitative Structure-Property relationship model for estimation of water solubility
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: DIBP
Temperature	not applicable
System	QSPR model using the Lu index, which is based on the shortest distance matrix.
pH	not applicable
Results Details Method	Predictive model developed using Lu index: Log Sw = 8.2431 - 0.5718 (Lu)
Standard Deviation Results	Not Reported
Results Details	n = 34; correlation coefficient (R) = 0.9869; standard error (SE) = 0.44; leave-one-out cross validation correlation coefficient (Rsv) = 0.9709; corresponding standarderrors (scv) = 0.47

EVALUATION

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	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	Uninformative	The QSPR model failed the standard error threshold of <0.3 and is therefore rated unacceptable.

Overall Quality Determination — Medium

Study Citation:	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.
OECD Harmonized Template:	Water Solubility
HERO ID:	5926117

EXTRACTION

Parameter	**Data**
Water Solubility	6.2 mg/L
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	24°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: Yalkowsky, S.H., He Yan, Jain, P. Handbook of Aqueous Solubility Data Second Edition. CRC Press, Boca Raton, FL 2010. p. 1111

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Diisobutyl phthalate. 84-69-5..
OECD Harmonized Template:	Water Solubility
HERO ID:	5926150

EXTRACTION

Parameter	**Data**
Water Solubility	6.2 mg/L
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	Unit conversion conducted to obtain 6.2 mg/L. Reported as 2.23e-5 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'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. Yalkowsky, SH and DannenFelser, RM (1992)

Study Citation:	CPSC, (2015). Exposure assessment: Composition, production, and use of phthalates.
OECD Harmonized Template:	Flash Point
HERO ID:	5155508

EXTRACTION

Parameter	**Data**
Flash Point	161 - 185 C
CASRN and Test Material	84-69-5; di-isobutyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; liquid; 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	The 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)	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 is from a publicly available secondary source without peer-review.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination Medium

* Related References: CPSC (U.S. Consumer Product Safety Commission). 2010. Review of Exposure Data and Assessments for Selected Dialkyl Ortho-Phthalates. CPSC-D-06-0006. Consumer Product Safety Commission, Bethesda, MD.

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 6782 Diisobutyl phthalate.
OECD Harmonized Template:	Flash Point
HERO ID:	6629592

EXTRACTION

Parameter	**Data**
Flash Point	385 F
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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

EVALUATION

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 secondary database with a reference to the original source.
	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: 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 Compound Summary for CID 6782 Diisobutyl phthalate.
OECD Harmonized Template:	Flash Point
HERO ID:	6629592

EXTRACTION

Parameter	**Data**
Flash Point	365 F
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	Open cup
Standard Deviation Results	Not reported
Results Details	185°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	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 secondary database with a reference to the original source.
	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, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.
OECD Harmonized Template:	Flash Point
HERO ID:	5926117

EXTRACTION

Parameter	**Data**
Flash Point	365 F
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	185°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. 325-47

Study Citation:	RSC, (2019). ChemSpider: Diisobutyl phthalate.
OECD Harmonized Template:	Flash Point
HERO ID:	5926262

EXTRACTION

Parameter	**Data**
Flash Point	169 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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: Diisobutyl phthalate.
OECD Harmonized Template:	Flash Point
HERO ID:	5926262

EXTRACTION

Parameter	**Data**
Flash Point	336.2 F
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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: Diisobutyl phthalate.
OECD Harmonized Template:	Flash Point
HERO ID:	5926262

EXTRACTION

Parameter	**Data**
Flash Point	180 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	185 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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:	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.
OECD Harmonized Template:	Autoflammability
HERO ID:	5926117

EXTRACTION

Parameter	**Data**
Auto-flammability	810 F
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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	432°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	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: National Fire Protection Association; Fire Protection Guide to Hazardous Materials. 14TH Edition, Quincy, MA 2010, p. 325-47

Study Citation:	Sigma-Aldrich, (2020). Diisobutyl phthalate safety data sheet.
OECD Harmonized Template:	Autoflammability
HERO ID:	6302634

EXTRACTION

Parameter	**Data**
Auto-flammability	423 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	None; not specified; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	No; Sigma-Aldrich; Liquid; $\leq$100%
System	Not reported
Standard Deviation Results	Not reported
Results Details	Auto-ignition temperature = 423°C (793°F) at 1013 hPA
Results Value	423°C

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data is reported for the target 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	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	Low	Data is from a known chemical supplier. The data are from a primary source without expert peer-review or an unknown secondary source without peer-review and 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 Low

Study Citation:	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.
OECD Harmonized Template:	Viscosity
HERO ID:	5926117

EXTRACTION

Parameter	**Data**
Viscosity	41
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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
Test Conditions	Not Reported
Standard Deviation Results	Not Reported
Results Details	41 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: Gerhartz, W. (exec Ed.) Ullmann's Encyclopedia of Industrial Chemistry. 5th Ed. Vol A1: Deerfield Beach, FL: VCH Publishers. p. VA20 193.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Refractive Index
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
Refractive Index	1.491
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported
Results Details Methods	Not Reported
Parameter	Wavelength: 589 nm

EVALUATION

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: Fischer et al.; Pharmazeutische Zentralhalle; vol. 105; (1966); p. 73,74,

Study Citation:	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.
OECD Harmonized Template:	Refractive Index
HERO ID:	5926117

EXTRACTION

Parameter	**Data**
Refractive Index	1.4900
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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
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	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: Lewis, R.J. Sr. 2007. Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY.

Study Citation:	RSC, (2019). ChemSpider: Diisobutyl phthalate.
OECD Harmonized Template:	Refractive Index
HERO ID:	5926262

EXTRACTION

Parameter	**Data**
Refractive Index	1.49
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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
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: Alfa Aesar

Study Citation:	Cousins, I., Mackay, D. (2000). Correlating the physical–chemical properties of phthalate esters using the 'three solubility' approach. Chemosphere 41(9):1389-1399.
OECD Harmonized Template:	Henry's Law
HERO ID:	4159647

EXTRACTION

Parameter	**Data**
Henry's Law	0.133 Pa m3/mol
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	None; QSAR; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: DIBP
Temperature	25°C
pH	Not reported
System	Three solubility approach: a quantitative structure-property relationship; correlations between apparent-solubilities of liquid state compounds in air and water, and molecular structures used to estimate partition coefficient Kaw (air-water)
Standard Deviation Results	Not reported
Results Details	log Kaw = -4.27
Results Details Methods	Not applicable

EVALUATION

Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are 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	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 AND the model performance was known and r2 $>$ 0.7, q2 $>$ 0.5, and SE $<$ 0.3.

Overall Quality Determination — High

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Henry's Law
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
Henry's Law	1.83E-7 atm-m3/mol
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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
pH	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported
Results Details Methods	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: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb.4; (1997); p. 667 - 749

Study Citation:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	Henry's Law
HERO ID:	3475635

EXTRACTION

Parameter	**Data**
Henry's Law	14.78 kPa
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate
Confidentiality, Type, and Guideline	None; Calculation; Non-guideline
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.
Temperature	298.15 K
pH	Not reported
System	Not reported
Standard Deviation Results	Not reported
Results Details	Reported as 14.78 kPa
Results Details Methods	Calculated based on experimental vapor pressure (0.0105 Pa) and mole fraction of water solubility (7.080 x 10^-7).

EVALUATION

Domain	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) [and/or] other 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	The analytical method is non-standard but is expected to be appropriate, based on methods used to derive calculation inputs.
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:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-370.
OECD Harmonized Template:	Henry's Law
HERO ID:	3475635

EXTRACTION

Parameter	**Data**
Henry's Law	10.77 Pa·m3/J
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate
Confidentiality, Type, and Guideline	None; Calculation; Non-guideline
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.
Temperature	298.15 K
pH	Not reported
System	Air-water partition coefficient Kaw; calculated using Henry's law constant based on experimental vapor pressure (0.0105 Pa) and mole fraction of water solubility (7.080 x 10^-7); WS: dynamic saturation method; VP: dynamic gas saturation method
Standard Deviation Results	Not reported
Results Details	Reported as 10.77 Pa·m3/J; Kaw = KhMw/RTρw (Kh: Henry's law constant; Mw: molar mass, R: gas constant, ρw: density of water)
Results Details Methods	experimental vapor pressure: HPLC-UV and water solubility: HPLC-UV (using an internal calibration method with BBP)

EVALUATION

Domain		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) [and/or] other 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	High	The analytical methods are 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 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:	Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173.
OECD Harmonized Template:	Henry's Law
HERO ID:	807140

EXTRACTION

Parameter	**Data**
Henry's Law	Not Reported
CASRN and Test Material	84-69-5; diisobutyl phthalate
Confidentiality, Type, and Guideline	none; QSAR; Quantitative Structure-Property relationship model for estimation of log Kaw
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: DIBP
Temperature	Not Reported
pH	Not Reported
System	Kaw = S(A)/Sw where S(A) is the solubility in air and Sw is the solubility in water
Standard Deviation Results	Not Reported
Results Details	Log Kaw= -4.30
Results Details Methods	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	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	Medium	Modeled data compared well to other data.

Overall Quality Determination Medium

Study Citation:	U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).
OECD Harmonized Template:	Henry's Law
HERO ID:	5155528

EXTRACTION

Parameter	**Data**
Henry's Law	6.43E-7 - atm-m^3/mole
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	No; not specified; NR
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	NR
pH	NR
System	Not Reported
Standard Deviation Results	NR
Results Details	NR
Results Details Methods	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	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other 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	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: Cites secondary source:NICNAS (National Industrial Chemicals Notification and Assessment Scheme). (2008) Diisobutyl phthalate. Existing chemical hazard assessment report. Australian Government. Available online athttp://www.nicnas.gov.au/Publications/CAR/Other/DiBPP%20hazard%20assessment.pdf (accessed October 13, 2010). HEROID 2316625

Study Citation:	U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).
OECD Harmonized Template:	Henry's Law
HERO ID:	5155528

EXTRACTION

Parameter	**Data**
Henry's Law	1.22E-06 - atm-m^3/mole
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	No; not specified; NR
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 deg C
pH	NR
System	Not Reported
Standard Deviation Results	NR
Results Details	NR
Results Details Methods	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	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other 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	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: Cites secondary source:HSDB (Hazardous Substance Data Bank). (2009) Diisobutyl phthalate. National Library of Medicine HSDB Database. (Last Revision, 01/05/2009).Same source but previous version of HEROID 5926117.Not previously extracted, HEROID in distiller.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..
OECD Harmonized Template:	Dielectric Constant
HERO ID:	5926421

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-69-5; Diisobutyl phthalate
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
Dielectric Constant	6.56
Temperature	25°C
System	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 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: Buchner; Barthel; Berichte der Bunsengesellschaft/Physical Chemistry Chemical Physics;vol. 101; nb. 10; (1997); p. 1509 - 1516

Study Citation:	Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173.
OECD Harmonized Template:	Other Properties
HERO ID:	807140

EXTRACTION

Parameter	**Data**
CASRN and Test Material	84-69-5; diisobutyl phthalate
Confidentiality, Type, and Guideline	none; QSAR; Quantitative Structure-Property relationship model for estimation of log Koa
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: DIBP
Results Value	Log Koa = 8.38
Results Details	Koa = So/S(A) where So is solubility in octanol and S(A) is the solubility in air
Results Remarks	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	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	Medium	Modeled data compared well to other data.

Overall Quality Determination — Medium

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