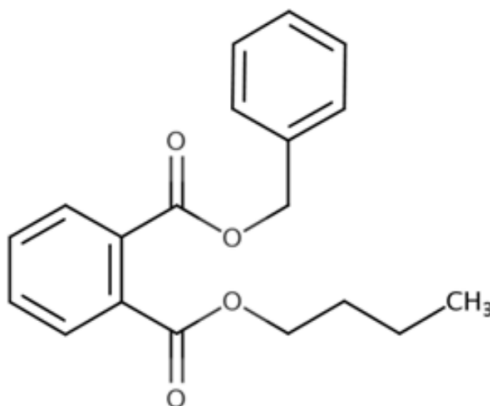

**Data Quality Evaluation and Data Extraction Information for
Physical and Chemical Properties for
Butyl benzyl phthalate (BBP)
(1,2-Benzenedicarboxylic acid, 1-butyl 2-(phenylmethyl) ester)**

Systematic Review Support Document for the Draft Risk Evaluation

CASRN: 85-68-7



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 Butyl Benzyl Phthalate (BBP)* 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 Butyl Benzyl Phthalate (BBP)*. 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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678590	NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP).	17
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5433544	Gobble, C., Chickos, J., Verevkin, S. P. (2014). Vapor pressures and vaporization enthalpies of a series of dialkyl phthalates by correlation gas chromatography. Journal of Chemical and Engineering Data 59(4):1353-1365.	79
679985	Howard, P. H., Banerjee, S., Robillard, K. H. (1985). Measurement of water solubilities octanol-water partition coefficients and vapor pressures of commercial phthalate esters. Environmental Toxicology and Chemistry 4(5):653-662.	80
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5433285	Ishak, H., Mokbel, I., Saab, J., Stephan, J., Paricaud, P., Jose, J., Goutaudier, C. (2019). Experimental measurements and thermodynamic modelling of aqueous solubilities, octanol-water partition coefficients and vapor pressures of dimethyl phthalate and butyl benzyl phthalate. Journal of Chemical Thermodynamics 131:286-293.	83
807140	Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173.	84
10225222	NIST, (2022). NIST Chemistry WebBook. Benzyl butyl phthalate (85-68-7). Standard Reference Database No. 69.	85
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654554	Mueller, M., Klein, W. (1992). Comparative evaluation of methods predicting water solubility for organic compounds. Chemosphere 25(6):769-782.	99
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1316095	Boese, B. L. (1984). Uptake efficiency of the gills of english sole (parophrys vetulus) for 4 phthalate esters. Canadian Journal of Fisheries and Aquatic Sciences 41(11):1713-1718.	109
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Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Physical Form or State
HERO ID:	3981013

EXTRACTION	
Parameter	Data
CASRN and Test Material	85-68-7; Butyl benzyl 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 Notes: NR
Results Value	liquid
Results Details	not specified

EVALUATION			
Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High
	Metric 2:	Appropriateness	High
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium
	Metric 4:	Reliability/Analytical Method	Low
Domain 3: Other	Metric 5:	Databases	High
	Metric 6:	Models	N/A

Overall Quality Determination

High

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

Study Citation:	EC/HC, (2000). Canadian environmental protection act priority substances list assessment report: Butylbenzylphthalate.
OECD Harmonized Template:	Physical Form or State
HERO ID:	1333728

EXTRACTION

Parameter	Data
CASRN and Test Material	85-68-7; Butylbenzylphthalate
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; a clear, oily liquid; Not Reported
Results Value	a clear, oily 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 (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3: Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4: Reliability/Analytical Method	Medium	The analytical method is 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: From: Howard, P.H., S. Banerjee and K.H. Robillard. 1985. Measurement of water solubilities, octanol/water partition coefficients and vapor pressure of commercial phthalate esters. Environ. Toxicol. Chem. 4: 653–661. HERO ID 82189

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	85-68-7; benzyl butyl 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	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: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

Study Citation:	ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Physical Form or State			
HERO ID:	2121719			
EXTRACTION				
Parameter	Data			
CASRN and Test Material	85-68-7; benzyl butyl 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; liquid; Not Reported			
Results Value	liquid			
Results Details	clear oily liquid w/slight characteristic odor and bitter taste			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7).
OECD Harmonized Template:	Physical Form or State
HERO ID:	5348378

EXTRACTION	
Parameter	Data
CASRN and Test Material	85-68-7; benzyl butyl 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; liquid; Not Reported
Results Value	liquid
Results Details	clear oily liquid w/slight characteristic odor and bitter taste

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

Overall Quality Determination	High
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Study Citation:	IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances.
OECD Harmonized Template:	Physical Form or State
HERO ID:	666726

EXTRACTION

Parameter	Data
CASRN and Test Material	85-68-7; benzyl butyl phthalate
Confidentiality, Type, and Guideline	none; not specified; NR
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; liquid; NR Notes: NR
Results Value	Clear, oily liquid
Results Details	NR

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Substance			
	Metric 1: Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2: Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties.
Domain 2: Test Reliability			
	Metric 3: Reliability/Unbiased (Method Objectivity)	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: Citing HERO ID 5185266

Study Citation:	IPCS, (1999). Concise international chemical assessment document 17: Butyl benzyl phthalate.
OECD Harmonized Template:	Physical Form or State
HERO ID:	675227

EXTRACTION	
Parameter	Data
CASRN and Test Material	85-68-7; Butyl benzyl phthalate
Confidentiality, Type, and Guideline	No; Not specified; NR
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; room temperature; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; liquid; Not Reported
Results Value	clear, oily 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
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Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.
OECD Harmonized Template:	Physical Form or State
HERO ID:	1239592

EXTRACTION	
Parameter	Data
CASRN and Test Material	85-68-7; butyl benzyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; liquid; NR
Results Value	a clear, oily liquid with a slight odor and a bitter taste
Results Details	Not Reported

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	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: Value added under HSDB (2015) HEROID: 5926116

Study Citation:	NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP).			
OECD Harmonized Template:	Physical Form or State			
HERO ID:	678590			
EXTRACTION				
Parameter	Data			
CASRN and Test Material	85-68-7; Butyl Benzyl Phthalate			
Confidentiality, Type, and Guideline	None; 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; liquid; Not Reported			
Results Value	clear, slightly 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’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	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:	Haynes, W. M. (2014). Butyl benzyl phthalate. :3-44.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5348395

EXTRACTION	
Parameter	Data
CASRN and Test Material	85-68-7; Benzyl butyl 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 recognized data collection where data are peer-reviewed by experts in the field.
	Metric 6: Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination	High
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Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926116

EXTRACTION

Parameter	Data
CASRN and Test Material	85-68-7; Benzyl butyl 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. 196.

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926116

EXTRACTION				
Parameter		Data		
CASRN and Test Material		85-68-7; Benzyl butyl 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		clear oil, liquid; slight odor		

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

Overall Quality Determination **High**

* Related References: Lewis, R.J. Sr. 2007. Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY. P. 196.

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

EXTRACTION

Parameter	Data
Melting Point	-35 - °C
CASRN and Test Material	85-68-7; Butyl benzyl phthalate
Confidentiality, Type, and Guideline	none; not specified; none
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Results Details Methods	not reported
Standard Deviation Results	not reported
Results Details	not reported

EVALUATION

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

Overall Quality Determination**High**

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

Study Citation:	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	< -35 °C
CASRN and Test Material	85-68-7; Benzylbutyl 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	not reported
Standard Deviation Results	not reported
Results Details	not reported

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

Overall Quality Determination

High

* Related References: Source cited: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

Study Citation:	ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Melting Point			
HERO ID:	2121719			
EXTRACTION				
Parameter	Data			
Melting Point	< -35 °C			
CASRN and Test Material	85-68-7; benzyl butyl 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	Data measured for a structural analogue of the subject chemical substance are consistent with what is expected for the subject chemical substance structural properties, features or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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: Citing Monsanto internal data (1988); Santicizer 160 bulletin. Monsanto Europe S.A., 8th edition.

Study Citation:	ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Melting Point			
HERO ID:	5348378			
EXTRACTION				
Parameter	Data			
Melting Point	< -35 °C			
CASRN and Test Material	85-68-7; benzyl butyl 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	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: Citing Monsanto internal data (1988); Santicizer 160 bulletin. Monsanto Europe S.A., 8th edition.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7..
OECD Harmonized Template:	Melting Point
HERO ID:	5926420

EXTRACTION

Parameter	Data
Melting Point	-35 °C
CASRN and Test Material	85-68-7; Benzyl butyl 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:	IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances.			
OECD Harmonized Template:	Melting Point			
HERO ID:	666726			
EXTRACTION				
Parameter	Data			
Melting Point	< −35 °C			
CASRN and Test Material	85-68-7; benzyl butyl phthalate			
Confidentiality, Type, and Guideline	none; not specified; NR			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Results Details Methods	NR			
Standard Deviation Results	NR			
Results Details	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 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 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: Citing HERO ID 5185266

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	Melting Point
HERO ID:	5926116

EXTRACTION

Parameter	Data
Melting Point	-35 °C
CASRN and Test Material	85-68-7; Benzyl butyl 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: David R.M. et al. 2012. Esters of Mono-, Di-, and Tricarboxylic Acids. Patty's Toxicology. 6th Ed. 199-2015. New York, NY: John Wiley & Sons, Inc.

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.
OECD Harmonized Template:	Melting Point
HERO ID:	1239592

EXTRACTION	
Parameter	Data
Melting Point	-35 °C
CASRN and Test Material	85-68-7; butyl benzyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	None; 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	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: Value added under HSDB (2015) HEROID: 5926116. Sax and Lewis (1989). Dangerous Properties of Industrial Materials. 7th. ed, pp. 41 1-412. Van Nostrand Reinhold, New York.

Study Citation:	NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP).
OECD Harmonized Template:	Melting Point
HERO ID:	678590

EXTRACTION	
Parameter	Data
Melting Point	-40.5 - °C
CASRN and Test Material	85-68-7; Butyl benzyl 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's physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

Medium

* Related References: Citing CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

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	370 - 377 C
CASRN and Test Material	85-68-7; benzyl 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; liquid; NR
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	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: IARC (International Agency for Research on Cancer), 1982. IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Some Industrial Chemicals and Dyestuffs. Vol. 29. International Agency for Research on Cancer. Lyon, France. Available at: <http://monographs.iarc.fr/ENG/Monographs/vol1-42/mono27.pdf>; 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:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Boiling Point
HERO ID:	3981013

EXTRACTION	
Parameter	Data
Boiling Point	370 - C
CASRN and Test Material	85-68-7; Butyl benzyl 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 Notes: NR
Standard Deviation Results	not reported
Results Details	@ 760 mm Hg

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

Overall Quality Determination

High

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

Study Citation:	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	370 C
CASRN and Test Material	85-68-7; Benzyl butyl 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	at 10.10 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	Medium	Measured data are consistent with the subject chemical substance structural features; appears to be a typo in the reporting of vapor pressure value.
Domain 2: Test Reliability	Metric 3: Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4: Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5: Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6: Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

Medium

* Related References: Source cited: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

Study Citation:	ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7).
OECD Harmonized Template:	Boiling Point
HERO ID:	2121719

EXTRACTION	
Parameter	Data
Boiling Point	370 - C
CASRN and Test Material	85-68-7; benzyl butyl 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
Standard Deviation Results	Not Reported
Results Details	10.10 hPa

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	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	Low	The data are from an MSDS without known expert 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: Citing Bayer AG MSDS Extract concerning physico chemical properties of BBP.

Study Citation:	ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7).
OECD Harmonized Template:	Boiling Point
HERO ID:	5348378

EXTRACTION	
Parameter	Data
Boiling Point	370 - C
CASRN and Test Material	85-68-7; benzyl butyl 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
Standard Deviation Results	Not Reported
Results Details	10.10 hPa

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	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	Low	The data are from an MSDS without known expert 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: Citing Bayer AG MSDS Extract concerning physico chemical properties of BBP.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926420

EXTRACTION

Parameter	Data
Boiling Point	250 C
CASRN and Test Material	85-68-7; Benzyl butyl 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	@ 22.5 torr

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1: 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: Haertel, Georg H.; Journal of Chemical and Engineering Data; vol. 30; nb. 1; (1985); p. 57 - 61

Study Citation:	Haynes, W. M. (2014). Butyl benzyl phthalate. :3-44.
OECD Harmonized Template:	Boiling Point
HERO ID:	5348395

EXTRACTION

Parameter	Data
Boiling Point	370 C
CASRN and Test Material	85-68-7; Benzyl butyl 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:	IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances.
OECD Harmonized Template:	Boiling Point
HERO ID:	666726

EXTRACTION

Parameter	Data
Boiling Point	370 C
CASRN and Test Material	85-68-7; benzyl butyl phthalate
Confidentiality, Type, and Guideline	none; not specified; NR
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Standard Deviation Results	NR
Results Details	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 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 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: Citing HERO ID 5185266

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926116

EXTRACTION

Parameter	Data
Boiling Point	370 C
CASRN and Test Material	85-68-7; Benzyl butyl 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. 2014. CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL.

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.
OECD Harmonized Template:	Boiling Point
HERO ID:	1239592

EXTRACTION	
Parameter	Data
Boiling Point	370 C
CASRN and Test Material	85-68-7; butyl benzyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; liquid; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION			
Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High
	Metric 2:	Appropriateness	High
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium
	Metric 4:	Reliability/Analytical Method	Medium
Domain 3: Other	Metric 5:	Databases	Medium
	Metric 6:	Models	N/A

Overall Quality Determination	Medium
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* Related References: Value added under HSDB (2015) HEROID: 5926116. Sax and Lewis (1989). Dangerous Properties of Industrial Materials. 7th. ed, pp. 41 1-412. Van Nostrand Reinhold, New York.

Study Citation:	NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP).
OECD Harmonized Template:	Boiling Point
HERO ID:	678590

EXTRACTION	
Parameter	Data
Boiling Point	370 - C
CASRN and Test Material	85-68-7; Butyl benzyl 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
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	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 CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

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

EXTRACTION

Parameter	Data
Boiling Point	370 C
CASRN and Test Material	85-68-7; Butyl benzyl 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 Notes: NR
Standard Deviation Results	NR
Results Details	Not Reported

EVALUATION

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

Overall Quality Determination**High**

Study Citation:	RSC, (2019). ChemSpider: Benzyl butyl phthalate.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926261

EXTRACTION	
Parameter	Data
Boiling Point	370 C
CASRN and Test Material	85-68-7; Benzyl butyl 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: Benzyl butyl phthalate.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926261			
EXTRACTION				
Parameter	Data			
Boiling Point	370 C			
CASRN and Test Material	85-68-7; Benzyl butyl 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:	U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7..			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926148			
EXTRACTION				
Parameter	Data			
Boiling Point	370 C			
CASRN and Test Material	85-68-7; Benzyl butyl 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 Benzyl butyl phthalate. 85-68-7..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926148

Parameter	Data
Boiling Point	370 C
CASRN and Test Material	85-68-7; Benzyl butyl 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

Domain	Metric	Rating	Comments
Domain 1: Substance			
	Metric 1: 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 Benzyl butyl phthalate. 85-68-7..			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926148			
EXTRACTION				
Parameter	Data			
Boiling Point	370 C			
CASRN and Test Material	85-68-7; Benzyl butyl 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 Benzyl butyl phthalate. 85-68-7..			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926148			
EXTRACTION				
Parameter	Data			
Boiling Point	370 C			
CASRN and Test Material	85-68-7; Benzyl butyl 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:	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	1.119 g/mL			
CASRN and Test Material	85-68-7; butyl benzyl 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	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.			
OECD Harmonized Template:	Density			
HERO ID:	3981013			
EXTRACTION				
Parameter	Data			
Density	1.116 -			
CASRN and Test Material	85-68-7; Butyl benzyl 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 Notes: NR			
Density Type	specific gravity (density of a substance divided by the density of water)			
System	not specified			
Temperature	25°C			
Standard Deviation Results	not reported			
Results Details	not reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	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:	Density
HERO ID:	7325405

EXTRACTION	
Parameter	Data
Density	1.116 g/cm3
CASRN and Test Material	85-68-7; Benzyl butyl 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
Density Type	relative density
System	not specified
Temperature	20°C
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: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

Study Citation:	ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Density			
HERO ID:	2121719			
EXTRACTION				
Parameter	Data			
Density	1.114 - 1.122 g/cm3			
CASRN and Test Material	85-68-7; benzyl butyl 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			
Density Type	density			
System	Not Reported			
Temperature	25°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: Citing Monsanto internal data (1988); Santicizer 160 bulletin. Monsanto Europe S.A., 8th edition.

Study Citation:	ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Density			
HERO ID:	5348378			
EXTRACTION				
Parameter	Data			
Density	1.114 - 1.122 g/cm3			
CASRN and Test Material	85-68-7; benzyl butyl 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			
Density Type	density			
System	Not Reported			
Temperature	25°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: Citing Monsanto internal data (1988); Santicizer 160 bulletin. Monsanto Europe S.A., 8th edition.

Study Citation:	IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances.
OECD Harmonized Template:	Density
HERO ID:	666726

EXTRACTION	
Parameter	Data
Density	1.1 g/cm3
CASRN and Test Material	85-68-7; benzyl butyl phthalate
Confidentiality, Type, and Guideline	none; not specified; NR
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Density Type	density
System	NR
Temperature	25°C
Standard Deviation Results	NR
Results Details	Not Reported

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	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: Citing HERO ID 5185266

Study Citation:	IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances.			
OECD Harmonized Template:	Density			
HERO ID:	666726			
EXTRACTION				
Parameter	Data			
Density	10.8			
CASRN and Test Material	85-68-7; benzyl butyl phthalate			
Confidentiality, Type, and Guideline	none; not specified; NR			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Density Type	relative vapor density			
System	NR			
Temperature	Not Reported			
Standard Deviation Results	NR			
Results Details	Air=1			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	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: Citing National Toxicology Program (1991) NTP Chemical Repository Data Sheet: Butyl BenzylPhthalate, Research Triangle Park, NC.

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.
OECD Harmonized Template:	Density
HERO ID:	1239592

EXTRACTION	
Parameter	Data
Density	1.116
CASRN and Test Material	85-68-7; butyl benzyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; liquid; NR
Density Type	specific gravity
System	NA
Temperature	25°C
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	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
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* Related References: Sax and Lewis (1989). Dangerous Properties of Industrial Materials. 7th. ed, pp. 41 1-412. Van Nostrand Reinhold, New York.

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.			
OECD Harmonized Template:	Density			
HERO ID:	1239592			
EXTRACTION				
Parameter	Data			
Density	10.8			
CASRN and Test Material	85-68-7; butyl benzyl phthalate			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	None; NR; liquid; NR			
Density Type	vapor density			
System	NA			
Temperature	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	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: Value added under HSDB (2015) HEROID: 5926116

Study Citation:	NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP).			
OECD Harmonized Template:	Density			
HERO ID:	678590			
EXTRACTION				
Parameter	Data			
Density	1.12 -			
CASRN and Test Material	85-68-7; Butyl Benzyl 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			
Density Type	Specific Gravity			
System	Not Reported			
Temperature	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	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 CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

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

EXTRACTION	
Parameter	Data
Density	1.111
CASRN and Test Material	85-68-7; butyl benzyl 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 Notes: NR
Density Type	density reported as specific gravity
System	NR
Temperature	25 deg C
Standard Deviation Results	NR
Results Details	Not Reported

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

Overall Quality Determination

High

Study Citation:	RSC, (2019). ChemSpider: Benzyl butyl phthalate.			
OECD Harmonized Template:	Density			
HERO ID:	5926261			
EXTRACTION				
Parameter	Data			
Density	1.119 g/mL			
CASRN and Test Material	85-68-7; Benzyl butyl phthalate			
Confidentiality, Type, and Guideline	none; experimental; not specified			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Density Type	density			
System	not specified			
Temperature	20°C			
Standard Deviation Results	Not reported			
Results Details	Not reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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: Cites: Merck Millipore

Study Citation:	RSC, (2019). ChemSpider: Benzyl butyl phthalate.			
OECD Harmonized Template:	Density			
HERO ID:	5926261			
Parameter		EXTRACTION		
Density		1.121 g/mL		
CASRN and Test Material		85-68-7; Benzyl butyl phthalate		
Confidentiality, Type, and Guideline		none; experimental; not specified		
Solvent, Reactivity, Storage, and Stability		NR; NR; NR; NR		
Radiolabel, Source, State, and Purity		NR; NR; NR; NR		
Density Type		density		
System		not specified		
Temperature		4°C		
Standard Deviation Results		Not reported		
Results Details		Not reported		
Domain		Metric		EVALUATION
				Rating
Domain 1: Substance				
	Metric 1:	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	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: Cites: Merck Millipore

Study Citation:	RSC, (2019). ChemSpider: Benzyl butyl phthalate.			
OECD Harmonized Template:	Density			
HERO ID:	5926261			
EXTRACTION				
Parameter	Data			
Density	1.1 g/mL			
CASRN and Test Material	85-68-7; Benzyl butyl phthalate			
Confidentiality, Type, and Guideline	none; experimental; not specified			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Density Type	density			
System	not specified			
Temperature	Not reported			
Standard Deviation Results	Not reported			
Results Details	Not reported			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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	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: Cites: Alfa Aesar

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7..
OECD Harmonized Template:	Density
HERO ID:	5926420

EXTRACTION

Parameter	Data
Density	1.118 g/cm3
CASRN and Test Material	85-68-7; Benzyl butyl 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; 2 values were reported in Reaxys; 1 value was reported as 1.118 at 20°C; 1 value was 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	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: Haertel, Georg H.; Journal of Chemical and Engineering Data; vol. 30; nb. 1; (1985); p. 57 - 61

Study Citation:	Haynes, W. M. (2014). Butyl benzyl phthalate. :3-44.
OECD Harmonized Template:	Density
HERO ID:	5348395

EXTRACTION

Parameter	Data
Density	1.119 g/cm3
CASRN and Test Material	85-68-7; Benzyl butyl 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
Standard Deviation Results	Not Reported
Results Details	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	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:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	Density
HERO ID:	5926116

EXTRACTION	
Parameter	Data
Density	1.119 g/cm3
CASRN and Test Material	85-68-7; Benzyl butyl 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
Standard Deviation Results	Not Reported
Results Details	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	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

High

* Related References: Haynes, W.M. (Ed.) 2014. CRC Handbook of Chemistry and Physics. 95th edition. CRC Press LLC, Boca Raton: FL.

Study Citation:	RSC, (2019). ChemSpider: Benzyl butyl phthalate.
OECD Harmonized Template:	Density
HERO ID:	5926261

EXTRACTION	
Parameter	Data
Density	1.1 g/cm ³
CASRN and Test Material	85-68-7; Benzyl butyl 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:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	Density
HERO ID:	5926116

EXTRACTION

Parameter	Data
Density	10.8
CASRN and Test Material	85-68-7; Benzyl butyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
System	Not reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	air = 1

EVALUATION

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

Overall Quality Determination**High**

* Related References: Lewis, R.J., Sr. (Ed.) 2012. Sax's Dangerous Properties of Industrial Materials. 12th edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. P. 501

Study Citation:	California Office of Environmental Health Hazard Assessment (OEHHA) (2013). Evidence on the carcinogenicity of butyl benzyl phthalate.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	5155605			
EXTRACTION				
Parameter	Data			
Vapor Pressure	8.55E-6 mm Hg			
CASRN and Test Material	85-68-7; Butyl benzyl phthalate			
Confidentiality, Type, and Guideline	No; not specified; NR			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	20°C			
System	NR			
Standard Deviation Results	NR			
Results Details	NR			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	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: No source cited; however, a similar value (8.6E-6 mm Hg) was reported in HERO IDs 1239592 and 5155508.

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	2.49x10-3 Pa			
CASRN and Test Material	85-68-7; butyl benzyl 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:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	3981013

EXTRACTION	
Parameter	Data
Vapor Pressure	8.25x10 ⁻⁶ - mm Hg
CASRN and Test Material	85-68-7; Butyl benzyl 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 Notes: NR
Temperature	25°C
System	not reported
Standard Deviation Results	not reported
Results Details	not reported

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

Overall Quality Determination

High

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

Study Citation:	EC/HC, (2000). Canadian environmental protection act priority substances list assessment report: Butylbenzylphthalate.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	1333728

EXTRACTION	
Parameter	Data
Vapor Pressure	1.15 mPa
CASRN and Test Material	85-68-7; Butylbenzylphthalate
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	20C
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is 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: From: Gledhill, W.E., R.G. Kaley, W.J. Adams, O. Hicks, P.R. Michael and V.W. Saeger. 1980. An environmental safety assessment of butylbenzyl phthalate. Environ. Sci. Technol. 14: 301–305. [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:	Vapor Pressure
HERO ID:	7325405

EXTRACTION

Parameter	Data
Vapor Pressure	0.00112 Pa
CASRN and Test Material	85-68-7; Benzyl butyl 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: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

Study Citation:	ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	2121719			
EXTRACTION				
Parameter	Data			
Vapor Pressure	0.00004 Pa			
CASRN and Test Material	85-68-7; benzyl butyl phthalate			
Confidentiality, Type, and Guideline	No; extrapolated; 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	20°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features 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: Citing Bayer AG (1987) Dampfdruckbestimmung von Unimol BB. Bayer AG, Leverkusen, den 07.11.87.

Study Citation:	ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	2121719			
EXTRACTION				
Parameter	Data			
Vapor Pressure	0.00799 Pa			
CASRN and Test Material	85-68-7; benzyl butyl 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°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features 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: Citing Mabey W.R. and T. Mill (1978) Critical review of hydrolysis of organic compounds in water under environmental conditions. J. Phys. Chem. Ref. Data 7, 383-415. HERO ID 9848.

Study Citation:	ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	2121719			
EXTRACTION				
Parameter	Data			
Vapor Pressure	0.5066 Pa			
CASRN and Test Material	85-68-7; benzyl butyl phthalate			
Confidentiality, Type, and Guideline	No; experimental; 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	20°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features 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	Low	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		

* Related References: Citing Bayer-Denmark in Monsanto (1988)

Study Citation:	ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	5348378			
EXTRACTION				
Parameter	Data			
Vapor Pressure	0.00004 Pa			
CASRN and Test Material	85-68-7; benzyl butyl phthalate			
Confidentiality, Type, and Guideline	No; extrapolated; 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	20°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features 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: Citing Bayer AG (1987) Dampfdruckbestimmung von Unimol BB. Bayer AG, Leverkusen, den 07.11.87.

Study Citation:	ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	5348378			
EXTRACTION				
Parameter	Data			
Vapor Pressure	0.00799 Pa			
CASRN and Test Material	85-68-7; benzyl butyl 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°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features 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: Citing Mabey W.R. and T. Mill (1978) Critical review of hydrolysis of organic compounds in water under environmental conditions. J. Phys. Chem. Ref. Data 7, 383-415. HERO ID 9848.

Study Citation:	ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7).
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5348378

EXTRACTION	
Parameter	Data
Vapor Pressure	0.5066 Pa
CASRN and Test Material	85-68-7; benzyl butyl phthalate
Confidentiality, Type, and Guideline	No; experimental; 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	20°C
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features 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	Low	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

* Related References: Citing Bayer-Denmark in Monsanto (1988)

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7..
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926420

EXTRACTION

Parameter	Data
Vapor Pressure	1.50015E-6 - 9.1E-5 mm Hg
CASRN and Test Material	85-68-7; Benzyl butyl 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	5 data points were reported in Reaxys; 4 values were reported at 1.50015E-6 to 9.1E-5 torr at standard temperature; 1 data point was outside the range, measured at non-standard or unreported temperatures.

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1: Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2: Appropriateness	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:	Gobble, C., Chickos, J., Verevkin, S. P. (2014). Vapor pressures and vaporization enthalpies of a series of dialkyl phthalates by correlation gas chromatography. Journal of Chemical and Engineering Data 59(4):1353-1365.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5433544

EXTRACTION	
Parameter	Data
Vapor Pressure	2.0E-4 Pa
CASRN and Test Material	85-68-7; Benzyl butyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	No; Aldrich; NR; Mass fraction: 0.99 Notes: Analytical standard: EPA 606-M phthalate ester mix. Source: Supelco.
Temperature	298.15 K
System	Correlation Gas Chromatography
Standard Deviation Results	Not specified; however, uncertainties in results were evaluated
Results Details	liquid phase vapor pressure. Manuscript authors erroneously omitted "-" from superscript in Table 19: "p·10 ⁶ /Pa" should be written as "p·10 ⁻⁶ /Pa". Same issue with Table 22.

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is 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	This metric is not applicable to this type of study.

Overall Quality Determination	High
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Study Citation:	Howard, P. H., Banerjee, S., Robillard, K. H. (1985). Measurement of water solubilities octanol-water partition coefficients and vapor pressures of commercial phthalate esters. Environmental Toxicology and Chemistry 4(5):653-662.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	679985

EXTRACTION

Parameter	Data
Vapor Pressure	1.1E-3 Pa
CASRN and Test Material	85-68-7; Butyl benzyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; If more than one manufacturer produced the individual PAE, the PAE product provided to us was an equal-proportion blend.
Radiolabel, Source, State, and Purity	NR; Provided to Chemical Manufacturers' Association by U.S. manufacturers.; NR; Each sample contained less than 1 % of non-PAE material, as determined by another laboratory. Notes: single isomer
Temperature	25°C
System	Measured by the gas saturation method: U.S. Environmental Protection Agency. 1980. Environmental test standards: Proposed rules. Vapor pressure. Fed. Reg. 45:77345-77350.
Standard Deviation Results	0.1E-3
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) and other physical/chemical properties.
Domain 2: Test Reliability	Metric 3: Reliability/Unbiased (Method Objectivity)	High	Peer-reviewed journal article with results compared to other literature values.
	Metric 4: Reliability/Analytical Method	High	Standard method used with experimental details reported.
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:	IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	666726			
EXTRACTION				
Parameter	Data			
Vapor Pressure	1.14 mPa			
CASRN and Test Material	85-68-7; benzyl butyl phthalate			
Confidentiality, Type, and Guideline	none; not specified; NR			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Temperature	20°C			
System	NR			
Standard Deviation Results	NR			
Results Details	NR			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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: Verschueren, 1996 HERO ID 5185266

Study Citation:	IPCS, (1999). Concise international chemical assessment document 17: Butyl benzyl phthalate.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	675227			
EXTRACTION				
Parameter	Data			
Vapor Pressure	0.1 - Pa			
CASRN and Test Material	85-68-7; Butyl benzyl 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	20°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	Medium	Measured data are higher than expected for 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		

Study Citation:	Ishak, H., Mokbel, I., Saab, J., Stephan, J., Paricaud, P., Jose, J., Goutaudier, C. (2019). Experimental measurements and thermodynamic modelling of aqueous solubilities, octanol-water partition coefficients and vapor pressures of dimethyl phthalate and butyl benzyl phthalate. Journal of Chemical Thermodynamics 131:286-293.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5433285

EXTRACTION	
Parameter	Data
Vapor Pressure	0.014 - 23.8 Pa
CASRN and Test Material	85-68-7; Butyl benzyl phthalate-BBP
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	None; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; NR; 0.98 (Supplier purity) Notes: Purity checked by GC >0.99
Temperature	343.15 K to 423.15 K
System	Test method: gas saturation method in absolute mode.
Standard Deviation Results	0.0005-0.45
Results Details	Several sources of uncertainty noted in using the saturation apparatus, especially for BBP with its very low vapor pressure.

EVALUATION				
Domain		Metric	Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Measured data are consistent with the subject chemical substance structural features. Not measured/reported for standard temperature.
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 likely to be appropriate based on comparison with peer-reviewed sources. Sources of uncertainty are noted in measuring very low vapor pressure.
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	1.27X10 ⁻³ Pa
CASRN and Test Material	85-68-7; butylbenzyl 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: BBzP
Temperature	Not Reported
System	Predictive model developed using gas law: $S(A) = P(\text{liquid substance})/RT$ where R= gas constant (8.314 Pa m ³ mol ⁻¹ K ⁻¹) and T = absolute temperature (298K); $\text{Log } S(A) = -0.2324 - 0.3215 (\text{Lu})$
Standard Deviation Results	Not Reported
Results Details	$\text{Log } S(A)$: 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 $r^2 > 0.7$, $q^2 > 0.5$, and $SE < 0.3$ (ECHA, 2016).

Overall Quality Determination
High

Study Citation:	NIST, (2022). NIST Chemistry WebBook. Benzyl butyl phthalate (85-68-7). Standard Reference Database No. 69.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	10225222

EXTRACTION

Parameter	Data
Vapor Pressure	Not Reported
CASRN and Test Material	85-68-7; Benzyl butyl phthalate
Confidentiality, Type, and Guideline	No; calculation; Calculated from the vapor pressure data reported by the method of least squares
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Temperature	431 K
System	NR
Standard Deviation Results	NR
Results Details	Enthalpy of vaporization = $\Delta v_{\text{apH}} = 89.0$ kJ/mol. Based on data from 416-516 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	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: Citing Stephenson, Richard M.; Malanowski, Stanislaw, Handbook of the Thermodynamics of Organic Compounds, 1987, <https://doi.org/10.1007/978-94-009-3173-2>.

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926116

EXTRACTION	
Parameter	Data
Vapor Pressure	8.25E-6 mm Hg
CASRN and Test Material	85-68-7; Benzyl butyl 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

EVALUATION			
Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1: 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: Howard, P.H. et al. 1985. Environ Tox Chem 4: 653-61.

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	1239592

EXTRACTION	
Parameter	Data
Vapor Pressure	8.6X10-6 mm Hg
CASRN and Test Material	85-68-7; butyl benzyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; liquid; NR
Temperature	20°C
System	Not Reported
Standard Deviation Results	NA
Results Details	Not Reported

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	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: Verschueren, (1983) (page missing from document); Hawley's, (1987). 11th ed. (N.I. Sax and R.J. Lewis, Sr., Eds.), p. 184. Van Nostrand Reinhold, New York.; Sax and Lewis, (1989). Dangerous Properties of Industrial Materials. 7th. ed, pp. 41 1-412. Van Nostrand Reinhold, New York.

Study Citation:	NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP).			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	678590			
EXTRACTION				
Parameter	Data			
Vapor Pressure	6x10^-7 - mm Hg			
CASRN and Test Material	85-68-7; Butyl Benzyl 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°C			
System	NR			
Standard Deviation Results	NA			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	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 CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7..
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926148

EXTRACTION	
Parameter	Data
Vapor Pressure	8.25E-6 mm Hg
CASRN and Test Material	85-68-7; Benzyl butyl 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

EVALUATION			
Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1: 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
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* Related References: PhysProp. Howard, PH et al. 1985

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}	4.70			
CASRN and Test Material	85-68-7; butyl benzyl 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:	EC/HC, (2000). Canadian environmental protection act priority substances list assessment report: Butylbenzylphthalate.
OECD Harmonized Template:	logKow
HERO ID:	1333728

EXTRACTION	
Parameter	Data
log k_{ow}	4.9
CASRN and Test Material	85-68-7; Butylbenzylphthalate
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 (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is 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: From: Leyder, F. and P. Boulanger. 1983. Ultraviolet absorption, aqueous solubility, and octanol–water partition coefficient for several phthalates. Bull. Environ. Contam. Toxicol. 30: 152–157. [no HERO ID]

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

EXTRACTION	
Parameter	Data
log k_{ow}	4.91
CASRN and Test Material	85-68-7; Dibutyl phthalate
Confidentiality, Type, and Guideline	none; experimental; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
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: ECHA c2007-2015b

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}	4.84
CASRN and Test Material	85-68-7; Benzyl butyl 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: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7..
OECD Harmonized Template:	logKow
HERO ID:	5926420

EXTRACTION	
Parameter	Data
log k_{ow}	4.77 - 4.84
CASRN and Test Material	85-68-7; Benzyl butyl 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; 4 values were reported in Reaxys; 2 values were reported in the range of 4.77 to 4.84 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: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb. 4; (1997); p. 667 - 749

Study Citation:	Howard, P. H., Banerjee, S., Robillard, K. H. (1985). Measurement of water solubilities octanol-water partition coefficients and vapor pressures of commercial phthalate esters. Environmental Toxicology and Chemistry 4(5):653-662.
OECD Harmonized Template:	logKow
HERO ID:	679985

EXTRACTION	
Parameter	Data
log k_{ow}	3.57
CASRN and Test Material	85-68-7; Butyl benzyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; If more than one manufacturer produced the individual PAE, the PAE product provided to us was an equal-proportion blend.
Radiolabel, Source, State, and Purity	NR; Provided to Chemical Manufacturers' Association by U.S. manufacturers.; NR; Each sample contained less than 1 % of non-PAE material, as determined by another laboratory. Notes: single isomer
Temperature	Not reported
System	HPLC method from a draft ASTM standard practice: Swann, R.L., D.A. Laskowski, P.J. McCall, K. Vander Kuy and H.J. Dishburger. 1983. Residue Rev. 85:17-28.
pH	Not reported
Results Details Method	The standards were benzene (log KOW=2.13), bromobenzene (log KOW = 2.99), biphenyl (log KO, = 3.76), bibenzyl (log KOW = 4.81), p,p-DDE (log KOW = 5.69), 2,4,5,2',5'-pentachlorobiphenyl (log KOW = 6.11) and 2,4,5,2',4',5'-hexachlorobiphenyl (log KOW = 6.72).
Standard Deviation Results	0
Results Details	Result is noted as being a log unit lower than other literature values.

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	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:	IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances.
OECD Harmonized Template:	logKow
HERO ID:	666726

EXTRACTION	
Parameter	Data
log k_{ow}	4.91 -
CASRN and Test Material	85-68-7; benzyl butyl phthalate
Confidentiality, Type, and Guideline	None; not specified; NR
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Temperature	NR
System	NR
pH	NR
Results Details Method	NR
Standard Deviation Results	NR
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: Citing HERO ID 5185266

Study Citation:	Ishak, H., Mokbel, I., Saab, J., Stephan, J., Paricaud, P., Jose, J., Goutaudier, C. (2019). Experimental measurements and thermodynamic modelling of aqueous solubilities, octanol-water partition coefficients and vapor pressures of dimethyl phthalate and butyl benzyl phthalate. Journal of Chemical Thermodynamics 131:286-293.
OECD Harmonized Template:	logKow
HERO ID:	5433285

EXTRACTION	
Parameter	Data
log k_{ow}	4.58
CASRN and Test Material	85-68-7; Butyl benzyl phthalate-BBP
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	None; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; NR; 0.98 (Supplier purity) Notes: Purity checked by GC >0.99
Temperature	298.15 K
System	Test method: static mode by using the shake-flask method. Volume proportion of octanol/water=1/8 for BBP.
pH	Not reported
Results Details Method	HPLC-UV; internal standard: dibutyl phthalate
Standard Deviation Results	Not Reported
Results Details	Measured at atmospheric pressure 0.1MPa (ca. 750 mm Hg);

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance.
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	Author reported the value is in good agreement (1-3.6% deviation) with two reported values and less so (11.4-15.3% deviation) with two reported values.
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:	logKow
HERO ID:	807140

EXTRACTION	
Parameter	Data
log k_{ow}	5.22
CASRN and Test Material	85-68-7; butylbenzyl 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: BBzP
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:	Mueller, M., Klein, W. (1992). Comparative evaluation of methods predicting water solubility for organic compounds. Chemosphere 25(6):769-782.			
OECD Harmonized Template:	logKow			
HERO ID:	654554			
EXTRACTION				
Parameter	Data			
log k _{ow}	4.87			
CASRN and Test Material	85-68-7; Benzyl butyl phthalate			
Confidentiality, Type, and Guideline	None; Calculation; 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	calculated Pow-values -MedChem-Software 1989			
EVALUATION				
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	Calculated data consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear.
	Metric 4:	Reliability/Analytical Method	N/A	This matrix is not applicable to this calculated data.
Domain 3: Other	Metric 5:	Databases	N/A	This matrix is not applicable to this calculated data.
	Metric 6:	Models	High	The model had a defined, unambiguous endpoint and the model performance was known.
Overall Quality Determination		High		

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	logKow
HERO ID:	5926116

EXTRACTION	
Parameter	Data
log k_{ow}	4.73
CASRN and Test Material	85-68-7; Benzyl butyl 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: Ellington, J.J.; Floyd, T.L.. 1996. Octanol/water partition coefficients for eight phthalate esters. EPA/600/S-96/006. Athens, GA: USEPA, National Exposure Research Lab.

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.			
OECD Harmonized Template:	logKow			
HERO ID:	1239592			
EXTRACTION				
Parameter	Data			
log k_{ow}	4.77			
CASRN and Test Material	85-68-7; butyl benzyl phthalate			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	None; 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	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	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: HEROID: 1337260 Gledhill et al (1980). An environmental safety assessment of butyl benzyl phthalate. Environ. Sci. Technol. 14, 301-305

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.			
OECD Harmonized Template:	logKow			
HERO ID:	1239592			
EXTRACTION				
Parameter	Data			
log k _{ow}	4.91			
CASRN and Test Material	85-68-7; butyl benzyl phthalate			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	None; 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	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	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: HEROID: 679764 Leyder and Boulanger (1983). Ultraviolet absorption, aqueous solubility, and octanol-water partition for several phthalates. Bull. Environ. Contam. Toxicol. 30, 152-157.

Study Citation:	NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP).			
OECD Harmonized Template:	logKow			
HERO ID:	678590			
EXTRACTION				
Parameter	Data			
log k_{ow}	4.59 -			
CASRN and Test Material	85-68-7; Butyl Benzyl 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’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Citing CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

Study Citation:	RSC, (2019). ChemSpider: Benzyl butyl phthalate.			
OECD Harmonized Template:	logKow			
HERO ID:	5926261			
EXTRACTION				
Parameter	Data			
log k_{ow}	3.388			
CASRN and Test Material	85-68-7; Benzyl butyl 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	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

Butyl benzyl phthalate

Study Citation:	SRC, (1984). Final report measurement of octanol-water partition coefficients of phthalate esters.			
OECD Harmonized Template:	logKow			
HERO ID:	1316207			
EXTRACTION				
Parameter	Data			
log k _{ow}	3.57 -			
CASRN and Test Material	85-68-7; butyl benzyl phthalate			
Confidentiality, Type, and Guideline	No; experimental; HPLC method			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; US Manufacturers; Not Reported; Not Reported Notes: analyzed to be within commercial specification limits			
Temperature	25°C			
System	partition coefficient correlated to HPLC retention time			
pH	Not reported			
Results Details Method	HPLC			
Standard Deviation Results	0			
Results Details	Author states the value is lower than most of the other reported or calculated values.			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Low	Calculated value is lower than expected.
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		Medium		

Study Citation:	U.S. EPA, (2017). Original BAF and BCF Data.			
OECD Harmonized Template:	logKow			
HERO ID:	3970058			
EXTRACTION				
Parameter	Data			
log k_{ow}	4.73			
CASRN and Test Material	85-68-7; Butyl benzyl 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 Notes: NR			
Temperature	NR			
System	NR			
pH	NR			
Results Details Method	NR			
Standard Deviation Results	NR			
Results Details	Mean log kow of 4.73 also reported as a calculated value.			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	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 HSDB (no year)

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7..			
OECD Harmonized Template:	logKow			
HERO ID:	5926148			
EXTRACTION				
Parameter	Data			
log <i>k_{ow}</i>	4.73			
CASRN and Test Material	85-68-7; Benzyl butyl 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. Ellington, JT and Floyd, TL. 1996

Study Citation:	Analytical Bio-Chemistry Labs, (1986). ABC final report - Method validation and water solubility for butyl benzyl phthalate analysis in well water.			
OECD Harmonized Template:	Water Solubility			
HERO ID:	1359224			
EXTRACTION				
Parameter	Data			
Water Solubility	2.5 - 2.8 ppm			
CASRN and Test Material	85-68-7; Butyl benzyl phthalate			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; room temp; NR			
Radiolabel, Source, State, and Purity	NR; Monsanto Co; Liquid; 100%			
Temperature	15-20°C			
System	Solubility in well water, sampling date 4/2/1985, 700 ft well at ABC Laboratories; devoid of O2 therefore passed through aeration reservoir			
pH	7.8-8.3			
Results Details Method	Solubility in well water with a hardness of 250 mg/L at a temp of 15 deg C = 2.6 ppm			
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)	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:	Boese, B. L. (1984). Uptake efficiency of the gills of english sole (parophrys vetulus) for 4 phthalate esters. Canadian Journal of Fisheries and Aquatic Sciences 41(11):1713-1718.
OECD Harmonized Template:	Water Solubility
HERO ID:	1316095

EXTRACTION	
Parameter	Data
Water Solubility	1.9 mg/L
CASRN and Test Material	85-68-7; BBP
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	12°C
System	Column generator method; seawater pumped through a sand column with the test substance.
pH	Not reported
Results Details Method	Extraction conducted with C18 Bond-Elut columns and eluted with ethylacetate, prior to electron capture capillary gas chromatography analysis.
Standard Deviation Results	Not Reported
Results Details	Determined for 25 o/oo seawater

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) and/or other physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	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	Analytic 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

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	3.8 mg/L			
CASRN and Test Material	85-68-7; butyl benzyl 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:	EC/HC, (2000). Canadian environmental protection act priority substances list assessment report: Butylbenzylphthalate.
OECD Harmonized Template:	Water Solubility
HERO ID:	1333728

EXTRACTION	
Parameter	Data
Water Solubility	2.69 mg/L
CASRN and Test Material	85-68-7; Butylbenzylphthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	water; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25C
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 (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is 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: From: Howard, P.H., S. Banerjee and K.H. Robillard. 1985. Measurement of water solubilities, octanol/water partition coefficients and vapor pressure of commercial phthalate esters. Environ. Toxicol. Chem. 4: 653–661. [HERO ID: 82189]

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

EXTRACTION	
Parameter	Data
Water Solubility	2.69 mg/L
CASRN and Test Material	85-68-7; butyl benzyl 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 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: ECHA c2007-2015b

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	2.9E3 ug/L			
CASRN and Test Material	Not Reported; BBP			
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	Data are measured or estimated for the subject chemical substance.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Hirzy, J.W., Adams, W.J., Gledhill, W.E. and Mieuse, J.P. (1979). Phthalates esters: the environmental issues. Unpublished document, Monsanto Industrial Chemicals Co. No HERO ID.

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	2.82E3 ug/L			
CASRN and Test Material	Not Reported; BBP			
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	2.69E3 ug/L			
CASRN and Test Material	Not Reported; BBP			
Confidentiality, Type, and Guideline	No; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	25 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 CMA (1983). Measurement of the water-solubility of phthalate esters. Final report, Contract PE-11. 0-WS-SRL. LI533-06, Syracuse Res. Corp., April, 1983. No HERO ID.

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	0.71E3 ug/L			
CASRN and Test Material	Not Reported; BBP			
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 nephotometric estimate of water solubility of highly 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	2.8 mg/L
CASRN and Test Material	85-68-7; Benzyl butyl 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	25-30°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: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

Study Citation:	ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Water Solubility			
HERO ID:	2121719			
EXTRACTION				
Parameter	Data			
Water Solubility	0.71 - 82.2 mg/L			
CASRN and Test Material	85-68-7; benzyl butyl phthalate			
Confidentiality, Type, and Guideline	No; experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
pH	Not Reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	collected from the literature			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	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: Citing Mackay, Shin and Ma (1994) Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals (volumes 2 and 3 are HERO ID 597912 and 5185256, respectively). Some values entered under HERO ID 679967 and 7401366.

Study Citation:	ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7).
OECD Harmonized Template:	Water Solubility
HERO ID:	5348378

EXTRACTION	
Parameter	Data
Water Solubility	0.71 - 82.2 mg/L
CASRN and Test Material	85-68-7; benzyl butyl phthalate
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	collected from the literature

EVALUATION			
Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1: 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: Citing Mackay, Shin and Ma (1994) Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals (volumes 2 and 3 are HERO ID 597912 and 5185256, respectively). Some values entered under HERO ID 679967 and 7401366.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7..
OECD Harmonized Template:	Water Solubility
HERO ID:	5926420

EXTRACTION	
Parameter	Data
Water Solubility	0.67 - 2.4 mg/L
CASRN and Test Material	85-68-7; Benzyl butyl 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 0.00067 to 0.0024 g/L at 25 C
Standard Deviation Results	Not Reported
Results Details	2 data points were reported in Reaxys; 2 values were reported at 0.00067 to 0.0024 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	0.710 mg/L
CASRN and Test Material	Not Reported; Benzylbutyl 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; NR; Liquid; NR
Radiolabel, Source, State, and Purity	24±2°C
Temperature	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.
System	Not reported
pH	Study performed at constant slit width, 3,2,2,3,5 slit arrangement. Excitation and emission monochromators set to 600 nm.
Results Details Method	Not Reported
Standard Deviation Results	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.
Results Details	

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	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:	Howard, P. H., Banerjee, S., Robillard, K. H. (1985). Measurement of water solubilities octanol-water partition coefficients and vapor pressures of commercial phthalate esters. Environmental Toxicology and Chemistry 4(5):653-662.
OECD Harmonized Template:	Water Solubility
HERO ID:	679985

EXTRACTION

Parameter	Data
Water Solubility	2.69 mg/L
CASRN and Test Material	85-68-7; Butyl benzyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; If more than one manufacturer produced the individual PAE, the PAE product provided to us was an equal-proportion blend.
Radiolabel, Source, State, and Purity	NR; Provided to Chemical Manufacturers' Association by U.S. manufacturers.; NR; Each sample contained less than 1 % of non-PAE material, as determined by another laboratory. Notes: single isomer
Temperature	25°C
System	Protocol was designed to meet or exceed the requirements of the EPA-recommended procedure stated in U.S. Environmental Protection Agency. 1979. TSCA premanufacture testing of new chemical substances: Water solubility. Fed. Reg. 44: 16253-16259.
pH	Not reported
Results Details Method	HPLC
Standard Deviation Results	0.15
Results Details	ASTM Type 2 water

EVALUATION

Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1: Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2: Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) and other physical/chemical properties.
Domain 2: Test Reliability	Metric 3: Reliability/Unbiased (Method Objectivity)	High	Standard test method used.
	Metric 4: Reliability/Analytical Method	High	Protocol was designed to meet or exceed the requirements of the EPA-recommended procedure.
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:	Howard, P. H., Banerjee, S., Robillard, K. H. (1985). Measurement of water solubilities octanol-water partition coefficients and vapor pressures of commercial phthalate esters. Environmental Toxicology and Chemistry 4(5):653-662.		
OECD Harmonized Template:	Water Solubility		
HERO ID:	679985		
		EVALUATION	
Domain	Metric	Rating	Comments

Study Citation:	Ishak, H., Mokbel, I., Saab, J., Stephan, J., Paricaud, P., Jose, J., Goutaudier, C. (2019). Experimental measurements and thermodynamic modelling of aqueous solubilities, octanol-water partition coefficients and vapor pressures of dimethyl phthalate and butyl benzyl phthalate. Journal of Chemical Thermodynamics 131:286-293.
OECD Harmonized Template:	Water Solubility
HERO ID:	5433285

EXTRACTION	
Parameter	Data
Water Solubility	1.3E-7 -
CASRN and Test Material	85-68-7; Butyl benzyl phthalate-BBP
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	None; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; NR; 0.98 (Supplier purity) Notes: Purity checked by GC >0.99
Temperature	298.15 K
System	Test method: dynamic saturation method.
pH	Not reported
Results Details Method	HPLC-UV
Standard Deviation Results	S = 3.95E-9, 95% confidence level
Results Details	Reported as mean aqueous solubility in mole fraction = 1.30E-7; Measured at 0.1 MPa (ca. 750 mm Hg)

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance. Author indicates value may be underestimated as it deviates more than 10% from literature values.
	Metric 2:	Appropriateness	Low	
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	Low	The analytical method is non-standard; great uncertainty was noted due to the difficulty of measuring very low aqueous solubility.
Domain 3: Other	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination**Medium**

Study Citation:	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	0.93 mg/L
CASRN and Test Material	85-68-7; butylbenzyl 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: BBzP
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:	Mueller, M., Klein, W. (1992). Comparative evaluation of methods predicting water solubility for organic compounds. Chemosphere 25(6):769-782.			
OECD Harmonized Template:	Water Solubility			
HERO ID:	654554			
EXTRACTION				
Parameter	Data			
Water Solubility	2.69 mg/L			
CASRN and Test Material	85-68-7; Benzyl butyl phthalate			
Confidentiality, Type, and Guideline	None; Calculation; 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	Statistical estimation in relation to partition coefficients.			
pH	Not reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Reported as 8.61E-6 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	Medium	Calculated data consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear.
	Metric 4:	Reliability/Analytical Method	N/A	This matrix is not applicable to this calculated data.
Domain 3: Other	Metric 5:	Databases	N/A	This matrix is not applicable to this calculated data.
	Metric 6:	Models	High	The model had a defined, unambiguous endpoint and the model performance was known.
Overall Quality Determination		High		

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	Water Solubility
HERO ID:	5926116

EXTRACTION	
Parameter	Data
Water Solubility	2.69 mg/L
CASRN and Test Material	85-68-7; Benzyl butyl 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	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: Howard, P.H. et al. 1985. Environ Tox Chem 4: 653-661.

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.
OECD Harmonized Template:	Water Solubility
HERO ID:	1239592

EXTRACTION	
Parameter	Data
Water Solubility	2.69 mg/L
CASRN and Test Material	85-68-7; butyl benzyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; liquid; NR
Temperature	20°C
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	almost insoluble in distilled water

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is 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
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* Related References: data entered in HEROID: 679985 Howard et al (1985)

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.			
OECD Harmonized Template:	Water Solubility			
HERO ID:	1239592			
EXTRACTION				
Parameter	Data			
Water Solubility	2.9 mg/L			
CASRN and Test Material	85-68-7; butyl benzyl phthalate			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	None; NR; liquid; NR			
Temperature	20C			
System	Not Reported			
pH	Not Reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	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: HEROID: 1337260 Gledhill et al (1980). An environmental safety assessment of butyl benzyl phthalate. Environ. Sci. Technol. 14, 301-305

Study Citation:	NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP).			
OECD Harmonized Template:	Water Solubility			
HERO ID:	678590			
EXTRACTION				
Parameter	Data			
Water Solubility	2.7 mg/L			
CASRN and Test Material	85-68-7; Butyl Benzyl 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	Reported as solubility in water: slight – 2.7 mg/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	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 CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

Study Citation:	SRC, (1983). Measurement of the water solubilities of phthalate esters (final report).
OECD Harmonized Template:	Water Solubility
HERO ID:	1316216

EXTRACTION	
Parameter	Data
Water Solubility	2.69 - mg/L
CASRN and Test Material	85-68-7; butyl benzyl phthalate
Confidentiality, Type, and Guideline	No; experimental; Measured test compound solubility in water by HPLC
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25°C
System	Samples shaken in distilled water, centrifuged and then analyzed
pH	Not Reported
Results Details Method	HPLC
Standard Deviation Results	±0.15
Results Details	The study reports that the experimental uncertainty exceeded that targeted in the SOP. Value reported based on curvilinear equation. Previously reported value = 2.83 ± 0.14 , value obtained by auditor = 2.88 ± 0.14 (linear equation).

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	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 study authors state that the experimental uncertainty exceeded that targeted in the SOP.
	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:	U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7..			
OECD Harmonized Template:	Water Solubility			
HERO ID:	5926148			
EXTRACTION				
Parameter	Data			
Water Solubility	2.69 mg/L			
CASRN and Test Material	85-68-7; Benzyl butyl 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 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. Howard, PH et al. 1985.

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 2347Benzyl butyl phthalate.
OECD Harmonized Template:	Flash Point
HERO ID:	6629530

EXTRACTION	
Parameter	Data
Flash Point	390 F
CASRN and Test Material	85-68-7; Benzyl 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; 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	Methodology was not reported in the secondary source. 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: 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 2347Benzyl butyl phthalate.			
OECD Harmonized Template:	Flash Point			
HERO ID:	6629530			
EXTRACTION				
Parameter	Data			
Flash Point	198 C			
CASRN and Test Material	85-68-7; Benzyl 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; 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	Methodology was not reported in the secondary source. 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, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	Flash Point
HERO ID:	5926116

EXTRACTION

Parameter	Data
Flash Point	390 F
CASRN and Test Material	85-68-7; Benzyl 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; NR; NR; NR
System	Closed cup
Standard Deviation Results	Not reported
Results Details	199°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 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**High**

* Related References: National Fire Protection Association; Fire Protection Guide to Hazardous Materials. 14TH Edition, Quincy, MA 2010, p. 325-18

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.			
OECD Harmonized Template:	Flash Point			
HERO ID:	1239592			
EXTRACTION				
Parameter	Data			
Flash Point	199 C			
CASRN and Test Material	85-68-7; butyl benzyl phthalate			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	None; 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	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: Value added under HSDB (2015) HEROID: 5926116

Study Citation:	RSC, (2019). ChemSpider: Benzyl butyl phthalate.
OECD Harmonized Template:	Flash Point
HERO ID:	5926261

EXTRACTION	
Parameter	Data
Flash Point	113 C
CASRN and Test Material	85-68-7; Benzyl butyl 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: Biosynth

Study Citation:	RSC, (2019). ChemSpider: Benzyl butyl phthalate.			
OECD Harmonized Template:	Flash Point			
HERO ID:	5926261			
EXTRACTION				
Parameter	Data			
Flash Point	230 F			
CASRN and Test Material	85-68-7; Benzyl butyl 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:	RSC, (2019). ChemSpider: Benzyl butyl phthalate.			
OECD Harmonized Template:	Flash Point			
HERO ID:	5926261			
EXTRACTION				
Parameter	Data			
Flash Point	110 C			
CASRN and Test Material	85-68-7; Benzyl butyl 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:	ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Autoflammability			
HERO ID:	2121719			
EXTRACTION				
Parameter	Data			
Auto-flammability	425 - C			
CASRN and Test Material	85-68-7; Butyl benzyl 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			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
Results Value	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Bayer AG, 1999 Final GLP Report, Determination of Safety-Relevant Data of Unimoll BB (no HERO ID). Value also under HERO ID 6629530.

Study Citation:	ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Autoflammability			
HERO ID:	5348378			
EXTRACTION				
Parameter	Data			
Auto-flammability	425 - C			
CASRN and Test Material	85-68-7; Butyl benzyl 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			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
Results Value	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Bayer AG, 1999 Final GLP Report, Determination of Safety-Relevant Data of Unimoll BB (no HERO ID). Value also under HERO ID 6629530.

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 2347Benzyl butyl phthalate.
OECD Harmonized Template:	Autoflammability
HERO ID:	6629530

EXTRACTION	
Parameter	Data
Auto-flammability	451 F
CASRN and Test Material	85-68-7; Benzyl 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; NR; NR; NR
System	Not reported
Standard Deviation Results	Not reported
Results Details	Not reported
Results Value	Not Reported

		EVALUATION		
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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: 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 2347Benzyl butyl phthalate.			
OECD Harmonized Template:	Autoflammability			
HERO ID:	6629530			
EXTRACTION				
Parameter	Data			
Auto-flammability	425 C			
CASRN and Test Material	85-68-7; Benzyl 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; NR; NR; NR			
System	Not reported			
Standard Deviation Results	Not reported			
Results Details	Not reported			
Results Value	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

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

Study Citation:	NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195.
OECD Harmonized Template:	Autoflammability
HERO ID:	1239592

EXTRACTION	
Parameter	Data
Auto-flammability	233 C
CASRN and Test Material	85-68-7; butyl benzyl phthalate
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; liquid; NR
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported
Results Value	Not Reported

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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: Verschueren, (1983) (page missing from document); Hawley's, (1987). 11th ed. (N.I. Sax and R.J. Lewis, Sr., Eds.), p. 184. Van Nostrand Reinhold, New York.; Sax and Lewis, (1989). Dangerous Properties of Industrial Materials. 7th. ed, pp. 41 1-412. Van Nostrand Reinhold, New York.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7..
OECD Harmonized Template:	Viscosity
HERO ID:	5926420

EXTRACTION

Parameter	Data
Viscosity	55
CASRN and Test Material	85-68-7; Benzyl butyl 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	At 20°C; 3 values were reported in Reaxys; 1 value was reported as 0.55 P at 20°C; 2 values were outside this range or measured at non-standard temperatures.

EVALUATION

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

Overall Quality Determination**High**

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

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7..
OECD Harmonized Template:	Refractive Index
HERO ID:	5926420

EXTRACTION	
Parameter	Data
Refractive Index	1.5356
CASRN and Test Material	85-68-7; Benzyl butyl 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	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 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
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* Related References: Fischer et al.; Pharmazeutische Zentralhalle; vol. 105; (1966); p. 73,74

Study Citation:	NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7.
OECD Harmonized Template:	Refractive Index
HERO ID:	5926116

EXTRACTION	
Parameter	Data
Refractive Index	1.535 - 1.540
CASRN and Test Material	85-68-7; Benzyl butyl 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: IARC. 1982. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer.

Study Citation:	RSC, (2019). ChemSpider: Benzyl butyl phthalate.			
OECD Harmonized Template:	Refractive Index			
HERO ID:	5926261			
EXTRACTION				
Parameter	Data			
Refractive Index	1.54			
CASRN and Test Material	85-68-7; Benzyl butyl 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	0.205 Pa m ³ /mol
CASRN and Test Material	85-68-7; Butylbenzyl 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: BBP
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 = -4.08
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 r ² > 0.7, q ² > 0.5, and SE < 0.3.

Overall Quality Determination

High

Study Citation:	EC/HC, (2000). Canadian environmental protection act priority substances list assessment report: Butylbenzylphthalate.
OECD Harmonized Template:	Henry's Law
HERO ID:	1333728

EXTRACTION

Parameter	Data
Henry's Law	0.133 Pa-m3/mol
CASRN and Test Material	85-68-7; Butylbenzylphthalate
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
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 substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3: Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4: Reliability/Analytical Method	Medium	The analytical method is 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: From: Lyman, W.J., W.F. Reehl and D.H. Rosenblatt.1982. Handbook on chemical property estimation methods. Environmental behaviour of organic compounds. McGraw-Hill, New York, N.Y. [cited in Howard, 1989] [HERO ID - 82189?]

Study Citation:	ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Henry’s Law			
HERO ID:	2121719			
EXTRACTION				
Parameter	Data			
Henry’s Law	0.176 - Pa.m3/mol			
CASRN and Test Material	85-68-7; Butyl benzyl phthalate			
Confidentiality, Type, and Guideline	No; Calculation; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
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 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	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		Medium		

Study Citation:	ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7).			
OECD Harmonized Template:	Henry’s Law			
HERO ID:	5348378			
EXTRACTION				
Parameter	Data			
Henry’s Law	0.176 - Pa.m3/mol			
CASRN and Test Material	85-68-7; Butyl benzyl phthalate			
Confidentiality, Type, and Guideline	No; Calculation; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
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	Calculated data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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		Medium		

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7..
OECD Harmonized Template:	Henry's Law
HERO ID:	5926420

EXTRACTION	
Parameter	Data
Henry's Law	7.61E-7 atm-m3/mol
CASRN and Test Material	85-68-7; Benzyl butyl 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	Reported as 0.077108 Pa-m3/mol
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:	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	85-68-7; butylbenzyl 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: BBzP
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= -3.76
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:	NICNAS, (2015). Priority existing chemical assessment report no. 40: Butyl benzyl phthalate.
OECD Harmonized Template:	Henry's Law
HERO ID:	3664467

EXTRACTION	
Parameter	Data
Henry's Law	1.28X10 ⁻⁴ - kPa m ³ /mol
CASRN and Test Material	85-68-7; butyl benzyl phthalate
Confidentiality, Type, and Guideline	No; not specified; NR
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Temperature	25°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 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	Low	Unable to confirm the value in the primary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

Low

* Related References: Citing ChemIDplus and ECB (2007) European Union Risk Assessment Report (EU RAR) on benzyl butyl phthalate (BBP), HERO ID 2121719. However, different values were reported in these cited sources.

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	85-68-7; butylbenzyl 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: BBzP
Results Value	Log Koa = 8.98
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
K _{oa}	Octanol-Air partition coefficient
K _{ow}	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
pK _a	Negative base 10 Log of Acid Dissociation Constant (K _a)
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