



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

Systematic Review Support Document for the Draft Risk Evaluation

CASRN: 84-69-5

$$H_3C$$
 CH_3
 CH_3

July 2025

PUBLIC RELEASE DRAFT July 2025

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

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5926421	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5	18
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Study Citation: OECD Harmonized		CPSC, (2015). Exposure assessment: Composition, production, and use of phthalates. Physical Form or State				
Template:	riiysicai roiiii (of State				
HERO ID:	5155508					
- ILEKO ID.	2122300		EXTEN A CONTO	A.,		
D		Data	EXTRACTIO	N		
Parameter		Data				
CLODAL LE LAC.		04.60.5 11.1 1.1 1.1 1.1				
CASRN and Test Material		84-69-5; di-isobutyl phthalate				
Confidentiality, Type, and		no; not specified; Not Reported				
Solvent, Reactivity, Storag	-	NR; NR; NR				
Radiolabel, Source, State,	and Purity	NR; NR; liquid; NR				
Results Value		Mostly odorless				
Results Details		Not Reported				
			EVALUATIO	N		
Domain		Metric	Rating	Comments		
Domain 1: Substance						
	Metric 1:	Representativeness	High	The information is related to the subject chemical substance.		
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.		
Domain 2: Test Reliabil	lity					
Domain 2. Test Renaon	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.		
	Medic 5.	(Method Objectivity)	1471	rading 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						
Domain 3: Other	Metric 5:	Databases	Medium	The date are forms a constant in horses had in mining		
				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 Quali	tv Determi	nation	High			
S , Crain Quain	c _j zecermin		8			

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

Study Citation:	ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the					
OECD Harmonized		Annex XV dossier proposing restrictions on four phthalates: Annexes. Physical Form or State				
Template:	,					
HERO ID:	7325405					
			EXTRACTIO)N		
Parameter		Data				
CASRN and Test Material		84-69-5; Di-isobutyl phthalate				
Confidentiality, Type, and	Guideline	none; not specified; not specified				
Solvent, Reactivity, Storag	ge, and Stability	NR; NR; NR; NR				
Radiolabel, Source, State,	and Purity	NR; NR; liquid; NR				
Results Value		Colourless liquid				
Results Details		Not Reported				
			EVALUATIO	N .		
Domain		Metric	Rating	Comments		
Domain 1: Substance						
	Metric 1:	Representativeness	High	Data 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 Reliabi	lity					
	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.		

^{*} Related References: Source cited: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Study Citation: Haz-Map, (2021). Hazardous agents: Diisobutyl phthalate.

OECD Harmonized Physical Form or State

Template:

HERO ID: 8486308

		EXTRACTIO
Parameter	Data	

CASRN and Test Material 84-69-5; Not Reported

Confidentiality, Type, and Guideline Not Reported; Not Reported; Not Reported

Solvent, Reactivity, Storage, and Stability

Not Reported; Not Reported;

Results Value Colorless viscous liquid

Results Details Not Reported

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data 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 Reliab	oility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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.

* Related References: Citing ICSC

U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).

Colorless, clear, mostly odorless, viscous liquid

Not Reported

OECD Harmonized Physical Form or State **Template: HERO ID:** 5155528 **EXTRACTION Parameter** Data CASRN and Test Material 84-69-5; Not Reported Confidentiality, Type, and Guideline None; Experimental; Not Reported Solvent, Reactivity, Storage, and Stability Not Reported; Not Reported; Not Reported Radiolabel, Source, State, and Purity Not Reported; Not Reported; Not Reported

			EVALUATIO	N
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 Reliab	bility			
	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

Study Citation:

Results Value

Results Details

High

^{*} Related References: Cites secondary sources:NICNAS (National Industrial Chemicals Notification and Assessment Scheme). (2008) Diisobutyl phthalate. Existing chemical hazard assessment report. Australian Government. Available online at: http://www.nicnas.gov.au/Publications/CAR/Other/DiBPP%20hazard%20assessment.pdf(accessed October 13, 2010). HEROID 5155528. ECHA (European Chemicals Agency). (2009) Annex IV Dossier, proposal for identification of a substance as SVHC/CMR (substances of very high concern/carcinogenic, mutagenic, or toxic to reproduction). http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdfHEROID unknown Not previously extracted. HEROID in distiller.

Study Citation: OECD Harmonized	NLM, (2013). l Physical Form	PubChem: Hazardous Substance Data Bar or State	nk: Diisobutyl pl	nthalate, 84-69-5.
Template: HERO ID:	5926117			
			EXTRACTIO	N
Parameter		Data		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and C	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	and Purity	Not Reported; NR; NR; NR		
Results Value		liquid		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
		(Method Objectivity)		
	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 Qualit	ty Determi	nation	High	

^{*} Related References: Lewis, R.J. Sr. 2007. Hawley's Condensed Chemical Dictionary. 15th Edition. John Wiley & Sons, Inc. New York, NY. P. 434.

HERO ID: 5926421 Table: 1 of 3

Study Citation: OECD Harmonized	Elsevier, (2019) Physical Form		ata for diisobutyl	phthalate. CAS Registry Number: 84-69-5
Template: HERO ID:	5926421			
			EXTRACTIO)N
Parameter		Data		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	Not Reported; NR; NR; NR		
Results Details		yellow		
			EVALUATIO	N
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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed database that contains references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	High	

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

Study Citation:

Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..

OECD Harmonized

ed Physical Form or State

Template: HERO ID:

D: 5926421

	EXTRACTION
Parameter	Data
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Results Details	colorless

			EVALUATIO	N
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 Reliab	ility			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
		(Method Objectivity)		
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a peer-reviewed database that contains references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

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

EXTRACTION

Diisobutyl Phthalate Physical Form or State HERO ID: 5926421 Table: 3 of 3

Study Citation:

Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..

OECD Harmonized Template:

ized Physical Form or State

Data

Template: HERO ID:

Parameter

5926421

CASRN and Test Material 84-69-5; Diisobutyl phthalate			
Confidentiality, Type, and Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR		
Results Details	red		
		EVALUATIO	N
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	N/A	Rating of this factor is not applicable to this kind of information.
	(Method Objectivity)		
Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other			
Metric 5:	Databases	High	Data is from a peer-reviewed database that contains references to the original sources.
Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
	••	***	
Overall Quality Determ	nination	High	

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

Study Citation: EC/HC, (2015). State of the science report: Phthalate substance grouping: Medium-chain phthalate esters: Chemical Abstracts Service Registry Numbers:

84-61-7; 84-64-0; 84-69-5; 523-31-9; 5334-09-8;16883-83-3; 27215-22-1; 27987-25-3; 68515-40-2; 71888-89-6.

OECD Harmonized Template:

Melting Point

HERO ID: 3688160

EXTRACTION			
Parameter	Data		
Melting Point	-52 °C		
CASRN and Test Material	84-69-5; diisobutyl phthalate		
Confidentiality, Type, and Guideline	no; experimental; not reported		
Solvent, Reactivity, Storage, and Stability	NR; NR; NR		
Radiolabel, Source, State, and Purity	NR; NR; liquid; NR		
Results Details Methods	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	Not Reported		

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

Overall Quality Determination

Medium

^{*} Related References: cites: European Chemicals Agency. c2007-2014b. substances database. [ECHA] Registered Search [cited CAS RN 84-69-5 [DIBP]. Helsinki (FI): ECHA. 2014 Sept] Available from: http://echa.europa.eu/information-on-chemicals/registeredsubstances; jsessionid=ADE5DCC9E32E9AC042ACD435168FEB84.live1?p_auth=UvS8Lp1d&p_p_id=registeredsubstances_WAR_regsubsportlet&p_p_lifecycle=1&p_p_state=normal&p_p_mode=v 1&p_p_col_pos=1&p_p_col_count=6&_registeredsubstances_WAR_regsubsportlet_javax.portlet.action=registeredSubstancesAction

Data -37 °C 84-69-5; Diisobutyl phthalate no; not specified; Not Reported ty NR; NR; NR; NR NR; NR; NR NR; NR; NR	EXTRACTIO	N
-37 °C 84-69-5; Diisobutyl phthalate no; not specified; Not Reported ty NR; NR; NR NR; NR; NR	EXTRACTIO	N
-37 °C 84-69-5; Diisobutyl phthalate no; not specified; Not Reported ty NR; NR; NR NR; NR; NR	EXTRACTIO	N
-37 °C 84-69-5; Diisobutyl phthalate no; not specified; Not Reported ty NR; NR; NR NR; NR; NR	EXTRACTIO	N
-37 °C 84-69-5; Diisobutyl phthalate no; not specified; Not Reported ty NR; NR; NR NR; NR; NR		
84-69-5; Diisobutyl phthalate no; not specified; Not Reported ty NR; NR; NR; NR NR; NR; liquid; NR		
84-69-5; Diisobutyl phthalate no; not specified; Not Reported ty NR; NR; NR; NR NR; NR; liquid; NR		
no; not specified; Not Reported ty NR; NR; NR; NR NR; NR; liquid; NR		
NR; NR; liquid; NR		
Not Reported		
1,013 hPa		
	EVALUATIO	N
Metric	Rating	Comments
Representativeness	High	Data are measured or estimated for the subject chemical substance.
Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
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.
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.
Models	N/A	Rating of this factor is not applicable to this kind of information.
	Databases Models ermination	. Models N/A

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

Study Citation:	ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes.			
OECD Harmonized	Melting Point	proposing resultations on roar pinning		
Template: HERO ID:	7325405			
			EXTRACTIO	N
Parameter		Data		
Melting Point		-37 °C		
CASRN and Test Material		84-69-5; Di-isobutyl phthalate		
Confidentiality, Type, and C	Guideline	none; not specified; not specified		
Solvent, Reactivity, Storage		NR; NR; NR		
Radiolabel, Source, State, a	•	NR; NR; liquid; NR		
Results Details Methods		at 1013 hPa		
Standard Deviation Results		not reported		
Results Details		not reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data 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 Reliabil	itv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Qualit	ty Determi	nation	High	

^{*} Related References: Source cited: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Study Citation: OECD Harmonized	Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5 Melting Point				
Template:					
HERO ID:	5926421				
]	EXTRACTIO	N	
Parameter		Data			
Melting Point		-58 °C			
CASRN and Test Material		84-69-5; Diisobutyl phthalate			
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, a	and Purity	Not Reported; NR; NR; NR			
Results Details Methods		Measured conditions were not reported.			
Standard Deviation Results	3	Not Reported			
Results Details		Not Reported			
			EVALUATIO	N	
Domain		Metric	Rating	Comments	
Domain 1: Substance					
	Metric 1:	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 Reliabil	ity				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Qualit	tv Determi	nation	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: OECD Harmonized	NLM, (2013). I Melting Point	PubChem: Hazardous Substance Data Ba	nk: Diisobutyl pl	nthalate, 84-69-5.
Template:	wiching I omit			
HERO ID:	5926117			
			EXTRACTIO	N
Parameter		Data		
Melting Point		-64 °C		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	Not Reported; NR; NR; NR		
Results Details Methods		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Quali	tv Determi	nation	High	
Over all Quali	ty Determin	เมลเเบม	mgn	

^{*} Related References: Clayton, G.D., Clayton, F.E. (Eds.) 1981. Patty's Industrial Hygiene and Toxicology: Volume 2A, 2B, 2C: Toxicology. 3rd Ed. New York: John Wiley Sons. P. 2345.

Study Citation: OECD Harmonized	RSC, (2019). C Melting Point	ChemSpider: Diisobutyl phthalate.		
Template: HERO ID:	5926262			
			EXTRACTION	
Parameter		Data		
Melting Point		-64 °C		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	Not Reported; NR; NR; NR		
Results Details Methods		Not Reported		
Standard Deviation Result	S	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 Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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.

^{*} Related References: Biosynth

Diisobutyl Phthalate Melting Point HERO ID: 5155528 Table: 1 of 2

Study Citation: OECD Harmonized	U.S. Consumer Melting Point	Product Safety Commission (CPSC) (201	1). Toxicity review of	of diisobutyl phthalate (DiBP, CASRN 84-69-5).
Template: HERO ID:	5155528			
			EXTRACTION	
Parameter		Data		
Melting Point		-50 - °C		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	No; not specified; NR		
Solvent, Reactivity, Storag	e, and Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Results Details Methods		Not Reported		
Standard Deviation Result	S	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 Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Quali	ty Determi	nation	Medium	

^{*} Related References: Cites secondary sources: European Commission. (2000) Substance ID: 84-69-5. Diisobutyl phthalate. IUCLID Dataset. European Commission. European Chemicals Bureau. Available online at http://ecb.jrc.ec.europa.eu/iuclid-datasheet/84695.pdf (accessed April 13, 2011). HEROID 680279

Diisobutyl Phthalate Melting Point HERO ID: 5155528 Table: 2 of 2

Study Citation:

U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).

OECD Harmonized

Melting Point

Template: HERO ID: 5	155528			
ILKO ID.	133320		EXTRACTION	
Parameter		Data	Zarracio rio: v	
Melting Point		-42 - °C		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guid	leline	No; not specified; NR		
Solvent, Reactivity, Storage, an	d Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State, and	Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Results Details Methods		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
N	letric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
N	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.
N	letric 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.
Ν	letric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

Medium

^{*} Related References: Cites secondary sources: European Commission. (2000) Substance ID: 84-69-5. Diisobutyl phthalate. IUCLID Dataset. European Commission. European Chemicals Bureau. Available online at http://ecb.jrc.ec.europa.eu/iuclid-datasheet/84695.pdf (accessed April 13, 2011). HEROID 680279

Study Citation: OECD Harmonized	U.S. EPA, (201 Melting Point	9). Chemistry Dashboard Information for	or Diisobutyl phthalate.	84-69-5
Template:	J			
HERO ID:	5926150			
			EXTRACTION	
Parameter		Data		
Melting Point		-64 °C		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage		NR; NR; NR		
Radiolabel, Source, State, a	-	Not Reported; NR; NR; NR		
Results Details Methods	•	Not Reported		
Standard Deviation Results	S	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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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				
Domain J. 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 Qualit	ty Determi	nation	Medium	

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

Diisobutyl Phthalate Melting Point HERO ID: 5926150 Table: 2 of 3

Study Citation:

U.S. EPA, (2019). Chemistry Dashboard Information for Diisobutyl phthalate. 84-69-5..

OECD Harmonized **Template:**

Melting Point

HERO ID: 5926150

		EXTRACTION	
Parameter	Data		
Melting Point	-64 °C		
CASRN and Test Material	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage, and Stability	NR; NR; NR		
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR		
Results Details Methods	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	Not Reported		
		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other			
Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

^{*} Related References: Alfa Aesar

Diisobutyl Phthalate Melting Point HERO ID: 5926150 Table: 3 of 3

Study Citation:

U.S. EPA, (2019). Chemistry Dashboard Information for Diisobutyl phthalate. 84-69-5..

OECD Harmonized

Melting Point

Template:

Template: HERO ID:	5926150			
			EXTRACTION	
Parameter		Data		
Melting Point		-64 °C		
CASRN and Test Materia	.1	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and		None; Experimental; Not Reported		
Solvent, Reactivity, Stora		NR; NR; NR		
Radiolabel, Source, State		Not Reported; NR; NR; NR		
Results Details Methods	, .	Not Reported		
Standard Deviation Resul	ts	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 Reliab	ility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Qual	ity Determi	nation	Medium	

^{*} Related References: Alfa Aesar

Diisobutyl Phthalate Melting Point HERO ID: 680451 Table: 1 of 1

Study Citation: Wang, L. M., Richert, R. (2007). Glass transition dynamics and boiling temperatures of molecular liquids and their isomers. Journal of Physical Chemistry

B 111(12):3201-3207.

OECD Harmonized

Melting Point

Template:

HERO ID: 680451

Parameter Data

Melting Point 191.1 K

CASRN and Test Material 84-69-5; Di-iso-butylphthalate
Confidentiality, Type, and Guideline None; Experimental; Not Reported

Solvent, Reactivity, Storage, and Stability NR; NR; Stable in temperature ranges to the glass transition temperature

Radiolabel, Source, State, and Purity NR; Aldrich; NR; 99%

Results Details Methods Not Reported Standard Deviation Results Not Reported

Results Details Value is a glass transition temperature.

			EVALUATIO:	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance's other physical/chemical properties.
Domain 2: Test Reliab	ility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	Data are from a peer-reviewed primary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ity Determ	ination	High	
Overall Quality Determination			mgn	

Study Citation: OECD Harmonized	CPSC, (2015). Boiling Point	Exposure assessment: Composition, pro	oduction, and use of phtl	halates.
Template:	5155500			
HERO ID:	5155508			
		_	EXTRACTION	
Parameter		Data		
Boiling Point		159 C		
CASRN and Test Material		84-69-5; di-isobutyl phthalate		
Confidentiality, Type, and		no; not specified; Not Reported		
Solvent, Reactivity, Storag		NR; NR; NR; NR		
Radiolabel, Source, State,	•	NR; NR; liquid; NR		
Standard Deviation Results	S	Not Reported		
Results Details		at 4 mm Hg		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	The data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with other physical properties.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		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 Quali	ty Determi	nation	Medium	

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

Study Citation:	ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes.				
OECD Harmonized	Boiling Point	sier proposing restrictions on four phina	nates: Annexes.		
Template:					
HERO ID:	7325405				
			EXTRACTIO	N	
Parameter		Data			
Boiling Point		320 C			
CASRN and Test Material		84-69-5; Di-isobutyl phthalate			
Confidentiality, Type, and	Guideline	none; not specified; not specified			
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State,	and Purity	NR; NR; liquid; NR			
Standard Deviation Results	S	not specified			
Results Details		not specified			
			EVALUATIO	N	
Domain		Metric	Rating	Comments	
Domain 1: Substance					
	Metric 1:	Representativeness	High	Data 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 Reliabil	lity				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Quali	ty Determi	nation	High		

^{*} Related References: Source cited: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Study Citation: OECD Harmonized	Elsevier, (2019) Boiling Point). Reaxys: physical-chemical property dat	ta for diisobutyl	phthalate. CAS Registry Number: 84-69-5
Template:	Doming 1 om			
HERO ID:	5926421			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		295 - 327 C		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	Not Reported; NR; NR; NR		
Standard Deviation Results	S	Not Reported		
Results Details		5 values were reported in Reaxys; 4 value pressure.	es were reported in	the range of 295 to 327 C at unreported pressures; 1 value was reported at non-standard
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Quali	ty Determi	nation	High	

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

Study Citation: OECD Harmonized	NIST, (2022). NIST Chemistry WebBook. 1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester (84-69-5). Standard Reference Database No. 69. Boiling Point				
Template: HERO ID:	10225182				
			EXTRACTIO	N	
Parameter		Data			
Boiling Point		593 - K			
CASRN and Test Material		84-69-5; Diisobutyl phthalate			
Confidentiality, Type, and C	Guideline	No; Not specified; NR			
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Repo	orted: Not Reported		
Radiolabel, Source, State, a	•	Not Reported; No			
Standard Deviation Results	•	Not Reported	rica, rioi reportea		
Results Details	•	Uncertainty assigned by TRC = 4. K			
			EVALUATIO	N	
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 Reliabil	itv				
20114111 27 1000 110014	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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					
Domain 3. Onici	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.	
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.	
Overall Quality Determination			Low		

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

Diisobutyl Phthalate Boiling Point HERO ID: 5926117 Table: 1 of 1

Study Citation: OECD Harmonized	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5. Boiling Point				
Template:	C				
HERO ID:	5926117				
			EXTRACTIO	N	
Parameter		Data			
Boiling Point		296.5 C			
CASRN and Test Material		84-69-5; Diisobutyl phthalate			
Confidentiality, Type, and		None; Experimental; Not Reported			
Solvent, Reactivity, Storage		NR; NR; NR; NR			
Radiolabel, Source, State, a	•	Not Reported; NR; NR; NR			
Standard Deviation Results	3	Not Reported			
Results Details		Not Reported			
			EVALUATIO	N	
Domain		Metric	Rating	Comments	
Domain 1: Substance					
	Metric 1:	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 Reliabil	itv				
Bomain 2. Test Remain	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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					
Domain 5: 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					

^{*} Related References: Haynes, W.M. (Ed.) 2010. CRC Handbook of Chemistry and Physics. 91st Edition. Boca Raton, FL: CRC Press Inc. p. 3-184.

Study Citation: OECD Harmonized	RSC, (2019). C Boiling Point	ChemSpider: Diisobutyl phthalate.		
Template: HERO ID:	5926262			
			EXTRACTION	
Parameter		Data		
Boiling Point		295.3 C		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage		NR; NR; NR		
Radiolabel, Source, State,	•	Not Reported; NR; NR; NR		
Standard Deviation Results	s	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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Quali	tv Determi	nation	Medium	

^{*} Related References: Biosynth

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

5926262

EXTR			

Parameter	Data
Boiling Point	327 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliab	ility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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: OECD Harmonized Rumble, J. R. (2018). Diisobutyl phthalate. :3-20.

Boiling Point

Template: HERO ID: 5926366			
		EXTRACTIO	N
Parameter	Data		
Boiling Point	296.5 C		
CASRN and Test Material	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage, and Stability	y NR; NR; NR		
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR		
Standard Deviation Results	Not Reported		
Results Details	Not Reported		
		EVALUATIO	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	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 Deter	rmination	High	

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

Boiling Point

Template:

			EXTRACTIO	N
Parameter		Data		
Boiling Point		296.5		
CASRN and Test Material		Not Reported; Di-isobutyl phthalate		
Confidentiality, Type, and Guideline		none; experimental; Not Reported		
Solvent, Reactivity, Storage, and Stability		NR; NR; NR; NR		
Radiolabel, Source, State, and Purity		NR; NR; NR; NR		
Standard Deviation Results		Not reported		
Results Details		Not reported		
			EVALUATIO	N
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				
1	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
]	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a known data-collection, prepared by experts in the field.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Study Citation: OECD Harmonized	U.S. EPA, (2019 Boiling Point	9). Chemistry Dashboard Information for	or Diisobutyl phth	alate. 84-69-5				
Template:	C							
HERO ID:	5926150							
EXTRACTION								
Parameter		Data						
Boiling Point		296 C						
CASRN and Test Material		84-69-5; Diisobutyl phthalate						
Confidentiality, Type, and		None; Experimental; Not Reported						
Solvent, Reactivity, Storage		NR; NR; NR; NR						
Radiolabel, Source, State, a	•	Not Reported; NR; NR; NR						
Standard Deviation Results	3	Not Reported						
Results Details		Not Reported						
EVALUATION								
Domain		Metric	Rating	Comments				
Domain 1: Substance		Wietric	Rating	Comments				
Domain 1. Substance	Metric 1:	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 Reliabil	•							
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.				
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.				
Domain 3: Other								
	Metric 5:	Databases	High	Data is from a publicly available database that provides references to the original, peer-reviewed source.				
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.				
Overall Quality Determination			High					

^{*} Related References: PhysProp

Study Citation:

U.S. EPA, (2019). Chemistry Dashboard Information for Diisobutyl phthalate. 84-69-5..

OECD Harmonized

Boiling Point

Template:

HERO ID: 5926150

EXTR	ACTION

Parameter	Data
Boiling Point	327 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR
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 Relial	bility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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

Diisobutyl Phthalate Boiling Point HERO ID: 5926150 Table: 3 of 3

Study Citation:

U.S. EPA, (2019). Chemistry Dashboard Information for Diisobutyl phthalate. 84-69-5..

OECD Harmonized

onized Boiling Point

Template: HERO ID:

D: 5926150

EXTRACTION				
	EXTR	ACT	IOI	V

Parameter	Data
Boiling Point	327 C
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	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 Relia	bility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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

Diisobutyl Phthalate Boiling Point HERO ID: 680451 Table: 1 of 1

Study Citation: Wang, L. M., Richert, R. (2007). Glass transition dynamics and boiling temperatures of molecular liquids and their isomers. Journal of Physical Chemistry

B 111(12):3201-3207.

OECD Harmonized

Boiling Point

Template:

HERO ID: 680451

EXT	'R A	C	ГT	ON	J

D 4	EATRACTION
Parameter	Data
Boiling Point	552 K
CASRN and Test Material	84-69-5; Di-iso-butylphthalate
Confidentiality, Type, and Guideline	None; Calculation; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; Stable in temperature ranges to the glass transition temperature
Radiolabel, Source, State, and Purity	NR; Aldrich; NR; 99%
Standard Deviation Results	Not Reported
Results Details	Boiling point calculated from experimentally derived relationship to measured glass transition temperature Tb = $132 + 2.2$ Tg (where Tg > 45 K). Tg = 191.1 K

			EVALUATIO:	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance's other physical/chemical properties.
Domain 2: Test Reliab	ility Metric 3:	Reliability/Unbiased	High	The methodology for producing the information is designed to answer a specific ques-
		(Method Objectivity)	111811	tion, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	Data are from a primary peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Study Citation:		Phthalate esters in foods: So	ources, occurrence, and analyt	tical methods. Comprehensive Reviews in Food Science and Food Safety
OECD Harmonized	9(1):21-43. Density			
Template:	Density			
HERO ID:	1322045			
			EXTRACTION	
Parameter		Data	EMIRICITON	
Density		1.039 g/mL		
CASRN and Test Material		84-69-5; di-iso-butyl phthalate		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage		NR; NR; NR		
Radiolabel, Source, State, a		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	3.6	D	TT: 1	
	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 Reliabil	itv			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		toward a particular outcome.
	Metric 4:	Reliability/Analytical Metho	od 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				
Domain J. Onloi	Metric 5:	Databases	Medium	The data are from a peer-reviewed secondary source without inclusion of references to the original sources.
	Metric 6:	Models	N/A	The metric is not applicable to the study type.
Overall Qualit	v Determina	ntion	Medium	

Diisobutyl Phthalate Density HERO ID: 3688160 Table: 1 of 1

Study Citation:	y Citation: EC/HC, (2015). State of the science report: Phthalate substance grouping: Medium-chain phthalate esters: Chemical Abstracts Service Registry Numb 84-61-7; 84-64-0; 84-69-5; 523-31-9; 5334-09-8;16883-83-3; 27215-22-1; 27987-25-3; 68515-40-2; 71888-89-6.			
OECD Harmonized	Density	-0, 04-09-3, 323-31-9, 3334-09-0,10003-	03-3, 27213-22-1, 279	707-25-5, 00515-40-2, 71000-07-0.
Template:	,			
HERO ID:	3688160			
			EXTRACTION	
Parameter		Data		
Density		1049 kg/m3		
CASRN and Test Material	l	84-69-5; diisobutyl phthalate		
Confidentiality, Type, and	Guideline	no; experimental; not specified		
Solvent, Reactivity, Storag	ge, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; liquid; NR		
Density Type		density		
System		Not Reported		
Temperature		not reported		
Standard Deviation Result	S	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 Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Quali	ty Determi	nation	Medium	

^{*} Related References: cites: Haynes WM, Lide DR. 2010. CRC Handbook of Chemistry and Physics. 91st edition.2010-2011. Boca Raton (FL): CRC Press, Taylor & Francis Group.

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

Template:

HERO ID: 5155528

		EXTRACTION
Parameter	Data	

Density 1.038 - g/cm3

CASRN and Test Material 84-69-5; Diisobutyl phthalate Confidentiality, Type, and Guideline None; not specified; NR

Solvent, Reactivity, Storage, and Stability NR; Not Reported; Not Reported

Radiolabel, Source, State, and Purity Not Reported; Not Reported; Not Reported; Not Reported

Density Type density
System NR
Temperature NR

Standard Deviation Results Not Reported

Results Details Reported as 1038 kg/m³

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

Overall Quality Determination Medium

^{*} Related References: Cites secondary sources:NICNAS (National Industrial Chemicals Notification and Assessment Scheme). (2008)Diisobutyl phthalate. Existing chemical hazard assessment report. Australian Government. Available online at http://www.nicnas.gov.au/Publications/CAR/Other/DiBPP%20hazard%20assessment.pdf(accessed October 13, 2010). HEROID 2316625 Not previously extracted, not in distiller.

Diisobutyl Phthalate Density HERO ID: 5155528 Table: 2 of 2

Study Citation:

U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).

OECD Harmonized

Density

Template: HERO ID:

		EXTRACTION	
Parameter	Data		
Density	1.037 - 1.049 g/cm3		
CASRN and Test Material	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	None; not specified; NR		
Solvent, Reactivity, Storage, and Stability	NR; Not Reported; Not Reported; Not Re	eported	
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Density Type	density	•	
System	NR		
Temperature	20 deg C		
Standard Deviation Results	Not Reported		
Results Details	Not Reported		
		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Substance		-	
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other			
Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determi		Medium	

^{*} Related References: Cites secondary sources: European Commission. (2000) Substance ID: 84-69-5. Diisobutyl phthalate. IUCLID Dataset. European Commission. European Chemicals Bureau. Available online at http://ecb.jrc.ec.europa.eu/iuclid-datasheet/84695.pdf (accessed April 13, 2011). HEROID 680279Not previously extracted, not in distiller.

Density). Reaxys: physical-chemical property data	a for diisobutyl _l	phthalate. CAS Registry Number: 84-69-5
5926421			
		EXTRACTIO	N
	Data		
	1.036 - 1.0412 g/cm3		
	84-69-5; Diisobutyl phthalate		
duideline	None; Experimental; Not Reported		
, and Stability	NR; NR; NR; NR		
nd Purity	Not Reported; NR; NR; NR		
	20°C		
	Not Reported		
	20°C; 3 values were reported in Reaxys; standard temperature.	2 values were rep	ported in the range of 1.036 to 1.0412 at 20°C; 1 value (1.049) was reported at a non-
		EVALUATIO	N
	Metric	Rating	Comments
	-		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.
ty			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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.
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.
	Metric 1: Metric 2: Metric 4:	Data 1.036 - 1.0412 g/cm3 84-69-5; Diisobutyl phthalate None; Experimental; Not Reported NR; NR; NR; NR Not Reported; NR; NR; NR 20°C Not Reported 20°C; 3 values were reported in Reaxys; standard temperature. Metric Metric 1: Representativeness Metric 2: Appropriateness Metric 3: Reliability/Unbiased (Method Objectivity) Metric 4: Reliability/Analytical Method Metric 5: Databases	EXTRACTIO Data 1.036 - 1.0412 g/cm3 84-69-5; Diisobutyl phthalate None; Experimental; Not Reported NR; NR; NR; NR Not Reported; NR; NR; NR 20°C Not Reported 20°C; 3 values were reported in Reaxys; 2 values were repstandard temperature. EVALUATIO Metric 1: Representativeness High Metric 2: Appropriateness N/A Metric 3: Reliability/Unbiased Medium (Method Objectivity) Metric 4: Reliability/Analytical Method Medium Metric 5: Databases High

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

Study Citation: OECD Harmonized	RSC, (2019). C Density	ChemSpider: Diisobutyl phthalate.		
Template:	-			
HERO ID:	5926262			
			EXTRACTION	
Parameter		Data		
Density		1.039 g/cm3		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storag		NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	Not Reported; NR; NR; NR		
Temperature		Not Reported		
Standard Deviation Results	S	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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Quali	tv Determi	nation	Medium	

^{*} Related References: Alfa Aesar

Study Citation:

Rumble, J. R. (2018). Diisobutyl phthalate. :3-20.

OECD Harmonized

Density

Template: HERO ID:

		EXTRACTIO)N
Parameter	Data		
Density	1.0490 g/cm3		
CASRN and Test Material	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR		
Temperature	15°C		
Standard Deviation Results	Not Reported		
Results Details	15°C		
		EVALUATIO	N
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		Metric	Kanng	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 Reliab	oility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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.

Study Citation: OECD Harmonized	NCBI, (2020). Density	PubChem Compound Summary for CID	6782 Diisobutyl	phthalate.
Template: HERO ID:	6629592			
			EXTRACTIO	N
Parameter		Data		
Density		9.59		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Not specified; Not specified		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
System		Not reported		
Temperature		Not Reported		
Standard Deviation Results	S	Not reported		
Results Details		Relative to air		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data reported for the target chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a secondary database with a reference to another database.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	ination	High	

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

Diisobutyl Phthalate Density HERO ID: 6629592 Table: 2 of 2

Study Citation: NCBI, (2020). PubChem Compound Summary for CID 6782 Diisobutyl phthalate.

OECD Harmonized Density

Template: 6629592

	EXTRACTION
Parameter	Data
Density	9.6
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	None; Not specified; Not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR
System	Not reported
Temperature	Not Reported
Standard Deviation Results	Not reported
Results Details	Air = 1

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

Overall Quality Determination High

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

Study Citation:	Cao, X. L. (2010) 9(1):21-43.	. Phthalate esters in foods: Sources,	occurrence, and analyt	tical methods. Comprehensive Reviews in Food Science and Food Safety
OECD Harmonized	Vapor Pressure			
Template: HERO ID:	1322045			
			EXTRACTION	
Parameter		Data		
Vapor Pressure		4.73x10-3 Pa		
CASRN and Test Material		84-69-5; di-iso-butyl phthalate		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	•	NR; NR; NR; NR		
Radiolabel, Source, State, a	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 Reliabili	ity			
	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 Qualit	ty Determina	ation	Medium	

Study Citation:	EC/HC, (2015). State of the science report: Phthalate substance grouping: Medium-chain phthalate esters: Chemical Abstracts Service Registry Nurs 84-61-7; 84-64-0; 84-69-5; 523-31-9; 5334-09-8;16883-83-3; 27215-22-1; 27987-25-3; 68515-40-2; 71888-89-6.				
OECD Harmonized Template:	Vapor Pressure	0,010,0,020010,000	00 0, 2, 210 22 1, 27	0, 20 0, 000 10 10 2, 7, 7, 1000 05 01	
HERO ID:	3688160				
			EXTRACTION		
Parameter		Data			
Vapor Pressure		6.3×10-3 Pa			
CASRN and Test Material		84-69-5; diisobutyl phthalate			
Confidentiality, Type, and	Guideline	no; experimental; not specified			
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, a	and Purity	NR; NR; liquid; NR			
Temperature		25°C			
System		Not Reported			
Standard Deviation Results	3	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 Reliabil	ity				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Qualit	tv Determi	nation	Medium		

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

Study Citation:		ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes.				
OECD Harmonized	Vapor Pressure		lates: Annexes.			
Template:	vapor i ressure					
HERO ID:	7325405					
	,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,		EXTEN A CONTO	A.,		
Danamatan		Data	EXTRACTIO	N		
Parameter		Data				
Vapor Pressure		0.01 Pa				
CASRN and Test Material		84-69-5; Di-isobutyl phthalate				
Confidentiality, Type, and	Guideline	none; not specified; not specified				
Solvent, Reactivity, Storage		NR; NR; NR				
Radiolabel, Source, State,	•	NR; NR; liquid; NR				
Temperature		20°C				
System		not specified				
Standard Deviation Results	S	not specified				
Results Details		not specified				
				A7		
Domain		3.4.4.	EVALUATIO:			
		Metric	Rating	Comments		
Domain 1: Substance	Metric 1:	Dammagantativanaga	High	Determined an estimated for the militate hands of the form		
	Metric 2:	Representativeness	High	Data 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 Reliabil	itv					
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased		
	M-4-:- 4.	(Method Objectivity)	Τ	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						
Zemain 3. Guici	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 Qualit	ty Dotormi	nation	High			
Overall Quali	iy Deteriiii	เเลเเบเเ	High			

^{*} Related References: Source cited: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Diisobutyl Phthalate Vapor Pressure HERO ID: 5926421 Table: 1 of 1

Study Citation: OECD Harmonized	Elsevier, (2019) Vapor Pressure	. Reaxys: physical-chemical property dat	ta for diisobutyl	ohthalate. CAS Registry Number: 84-69-5
Template: HERO ID:	5926421			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		2E-6 - 5.8E-4 mm Hg		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and C	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR		
Radiolabel, Source, State, a	and Purity	Not Reported; NR; NR; NR		
Temperature		25°C		
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		2 data points were reported in Reaxys; 2	values were report	ed at 2E-6 to 5.8E-4 torr at 25°C.
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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				
Domain J. Oulei	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 Qualit	ty Determi	nation	High	

^{*} Related References: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb. 4; (1997); p. 667 - 749

Study Citation:

Haz-Map, (2021). Hazardous agents: Diisobutyl phthalate.

OECD Harmonized

Vapor Pressure

HERO ID:	8486308			
			EXTRACTION	
Parameter		Data		
Vapor Pressure		= 0.00665 mm Hg		
CASRN and Test Mater	rial	84-69-5; Di-isobutyl phthalate		
Confidentiality, Type, a	nd Guideline	none; not specified; Not Reported		
Solvent, Reactivity, Sto		Not Reported; Not Reported; Not Reporte	d; Not Reported	
Radiolabel, Source, Sta	-	Not Reported; Not Reported; Not Reporte	-	
Temperature	·	not specified	•	
System		not specified		
Standard Deviation Res	ults	not specified		
Results Details		not specified		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance	<u> </u>		Tuung	- Commons
	Metric 1:	Representativeness	High	Data 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 Relia	ability			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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.

Study Citation:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition	on

coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-

OECD Harmonized

Template:

Results Details

370. Vapor Pressure

HERO ID: 3475635

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

Value is extrapolated from vapor pressures measured between 313.15 K and 423.15 K.

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups).
Domain 2: Test Reliab	oility			
	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.

Diisobutyl Phthalate Vapor Pressure HERO ID: 807140 Table: 1 of 1

Study Citation: Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology

83(2):168-173.

OECD Harmonized Template:

Vapor Pressure

HERO ID: 807140

EXTRACTION

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

			EVALUATIO	N
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 Reliabi	ility			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
		(Method Objectivity)		
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	High	The model had a defined, unambiguous endpoint AND the model performance was known and $r2 > 0.7$, $q2 > 0.5$, and $SE < 0.3$ (ECHA, 2016).

Overall Quality Determination High

Study Citation: OECD Harmonized	NLM, (2013). I Vapor Pressure	PubChem: Hazardous Substance Data Bar	nk: Diisobutyl pl	nthalate, 84-69-5.
Template: HERO ID:	5926117			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		4.76E-5 mm Hg		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	Not Reported; NR; NR; NR		
Temperature		25°C		
System		Not Reported		
Standard Deviation Result	S	Not Reported		
Results Details		from experimentally derived coefficients		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	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 Reliabi	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	Metric 4:	(Method Objectivity) Reliability/Analytical Method	Medium	towards a particular product or outcome. Analytical method is unknown but is likely to be appropriate based on the data's inclu-

sion in a peer-reviewed/recognized database or other secondary source.

Rating of this factor is not applicable to this kind of information.

Data is from a publicly available, peer-reviewed database that provides references to

Domain 3: Other

Metric 5:

Metric 6:

Overall Quality Determination

Databases

Models

High

N/A

High

original sources.

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

Study Citation:	Cao, X. L. (2010). 9(1):21-43.). Phthalate esters in foods: Sources, occurrence, and analytical methods. Comprehensive Reviews in Food Science and Food Safety			
OECD Harmonized	9(1):21-43. logKow				
Template:	8				
HERO ID:	1322045				
			EXTRACTION		
Parameter		Data			
$\log k_{ow}$		4.27			
CASRN and Test Material		84-69-5; di-iso-butyl phthalate			
Confidentiality, Type, and	Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage		NR; NR; NR			
Radiolabel, Source, State, a		NR; NR; NR			
Temperature	.	25°C			
System		Not Reported			
рH		Not Reported			
Results Details Method		Not Reported			
Standard Deviation Results	į.	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 Reliabil	itv				
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased	
		(Method Objectivity)		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					
_ small of 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 Qualit	ty Determina	ation	Medium		

Study Citation:		ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes.				
OECD Harmonized	logKow	sier proposing restrictions on four phinar	lates. Affilexes.			
Template:						
HERO ID:	7325405					
			EXTRACTIO	N		
Parameter		Data				
log k _{ow}	1	4.11				
CASRN and Test Materia		84-69-5; Di-isobutyl phthalate				
Confidentiality, Type, and Guideline		none; not specified; not specified NR; NR; NR; NR				
Solvent, Reactivity, Storage, and Stability 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 Result	ts	not specified				
Results Details		not specified				
			EVALUATIO			
Domain		Metric	Rating	Comments		
Domain 1: Substance						
	Metric 1:	Representativeness	High	Data 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 Reliab	ility					
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased		
		(Method Objectivity)		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						
Domain 5. Guiei	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are		
			8	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.		
0 110 11	. D.	4.	TT. 1			
Overall Quali	ity Determi	nation	High			

^{*} Related References: Source cited: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5..

OECD Harmonized	logKow). Reaxys. physical-elemical property date	a for unsobutyr	phulatate. Cris registry rumber. 64-67-5
Template: HERO ID:	5926421			
			EXTRACTIO	N
Parameter		Data		
$\log k_{ow}$		4.31 - 4.86		
CASRN and Test Material	1	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storag	ge, and Stability	NR; NR; NR		
Radiolabel, Source, State,	and Purity	Not Reported; NR; NR; NR		
Temperature		Not Reported		
System		Not Reported		
pН		Not Reported		
Results Details Method		Not Reported		
Standard Deviation Result	S	Not Reported		
Results Details		@ 25 C; 5 values were reported in Reaxy	rs; 3 values were re	eported at 4.31 to 4.86 at 25 C; 2 values were reported at unreported temperatures.
			EVALUATIO	N .
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	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 Reliabi	lity			
Domain 2. Test Kenaui	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	IVICUIC J.	Renaumty/Unutaseu	Mediulli	There is no indication that the methodology for producing the information was biased

Medium

High

N/A

Analytical method is unknown but is likely to be appropriate based on the data's inclu-

Data is from a secondary database with a references to the peer-reviewed original

sion in a peer-reviewed/recognized database or other secondary source.

Rating of this factor is not applicable to this kind of information.

towards a particular product or outcome.

Overall Quality Determination High

Databases

Models

(Method Objectivity)

Reliability/Analytical Method

Metric 4:

Metric 5:

Metric 6:

Study Citation:

Domain 3: Other

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

Study Citation: Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition

coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-

370. logKow

OECD Harmonized

Template:

HERO ID: 3475635

FXTR	۸,	C	rt/	N	

Parameter	Data
$\log k_{ow}$	4.34
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.
Temperature	298.15 K
System	Shake-flask method with n-octanol and purified water, quantified by HPLC-UV.
pH	Not reported
Results Details Method	n-Octanol pre-saturated water with the test substance is poured into a test vessel and stirred with a magnetic stirring bar. 100 g of the aqueous phase is analyzed through C-18 cartridges and eluted with methanol. The concentration of the solute is then quantified by HPLC-UV.
Standard Deviation Results	0.082
Results Details	Value the average of 3 replicates at atmospheric pressure.

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance	;			
	Metric 1:	Representativeness	High	Data 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 Relia	bility			
	Metric 3:	Reliability/Unbiased	High	The methodology for producing the information is designed to answer a specific ques-
		(Method Objectivity)		tion, and the methodology's objective is clear. Methodology reported in J. Saab, G.
	Metric 4:	Reliability/Analytical Method	Medium	Basil, R. About Niccol, J. Stephan, I. Mokbel, J. Jose, Chemosphere 82 (2011) 929-934. 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

PUBLIC RELEASE DRAFT July 2025

Diisobutyl Phthalate logKow HERO ID: 3475635 Table: 1 of 1

... continued from previous page

Study Citation: Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition

coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-

370. logKow

OECD Harmonized

Template: HERO ID:

		EVALUATION		
Domain	Metric	Rating	Comments	

Study Citation: Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology

83(2):168-173.

OECD Harmonized

logKow

Template:

HERO ID: 807140

EXTR	AC'	$\Gamma \mathbf{I} C$	N

	EATRACTION
Parameter	Data
$\log k_{ow}$	4.08
CASRN and Test Material	84-69-5; diisobutyl phthalate
Confidentiality, Type, and Guideline	none; QSAR; Quantitative Structure-Property relationship model for estimation of log Kow
Solvent, Reactivity, Storage, and Stability	NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR Notes: DIBP
Temperature	not applicable
System	QSPR model using the Lu index, which is based on the shortest distance matrix.
pН	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 Reliab	ility			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
		(Method Objectivity)		
	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: OECD Harmonized Template:	NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5. logKow				
HERO ID:	5926117				
			EXTRACTIO	N	
Parameter		Data			
$\log k_{ow}$		4.11			
CASRN and Test Material		84-69-5; Diisobutyl phthalate			
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, a	and Purity	Not Reported; NR; NR; NR			
Temperature		Not Reported			
System		Not Reported			
pH		Not Reported			
Results Details Method		Not Reported			
Standard Deviation Results	3	Not Reported			
Results Details		Not Reported			
			EVALUATIO	N	
Domain		Metric	Rating	Comments	
Domain 1: Substance					
	Metric 1:	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 Reliabil	ity				
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased	
		(Method Objectivity)		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 Qualit	ty Determi	nation	High		

^{*} Related References: Hansch, C., Leo, A., D. Hoekman. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society, 1995, p. 144

U.S. EPA, (2019). Chemistry Dashboard Information for Diisobutyl phthalate. 84-69-5..

OECD Harmonized	rmonized logKow		
Template:	C		
HERO ID:	5926150		
		EXTRACTION	
Parameter		Data	
log k _{ow}		4.11	
CASRN and Test Material		84-69-5; Diisobutyl phthalate	
Confidentiality, Type, and C	Guideline	None; Experimental; Not Reported	
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR	
Radiolabel, Source, State, a	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	

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance	e			
	Metric 1:	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 Relia	ability			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Qua	lity Determ	ination	High	

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

Study Citation:

Study Citation: OECD Harmonized Aktiengesellschaft,, BASF (2001). [Redacted] Physico-chemical properties of "Palatinol IC".

Water Solubility

Template:

HERO ID: 11182936

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

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

Study Citation:	Cao, X. L. (2010). Phthalate esters in foods: Sources, occurren	ce, and analytical methods.	. Comprehensive Reviews in Food Science and Food Safety
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OECD Harmonized

9(1):21-43. Water Solubility

Template: HERO ID:

		EXTRACTION	
Parameter	Data		
Water Solubility	9.9 mg/L		
CASRN and Test Material	84-69-5; di-iso-butyl phthalate		
Confidentiality, Type, and Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, and Purity	NR; NR; NR; NR		
Temperature	25°C		
System	Not Reported		
pH	Not Reported		
Results Details Method	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	Not Reported		
		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Substance		8	
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.
	Models	N/A	Rating of this factor is not applicable to this kind of information.

Study Citation: OECD Harmonized	CPSC, (2015). Water Solubilit	Exposure assessment: Composition, pro	duction, and use of pht	halates.
Template: HERO ID:	5155508			
пекотр:	3133308		EXTED A CITION	
Parameter		Data	EXTRACTION	
rarameter		Data		
Water Solubility		1.1x10-3 g/L		
CASRN and Test Material		84-69-5; di-isobutyl phthalate		
Confidentiality, Type, and	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	and Purity	NR; NR; liquid; NR		
Temperature		Not Reported		
System		Not Reported		
pH		Not Reported		
Results Details Method		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	The data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with other physical chemical properties.
Domain 2: Test Reliabil	ity			
Domain 2. Test Rendon	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	Wictife 5.	(Method Objectivity)	Wicdium	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				
Domain J. Onici	Metric 5:	Databases	Medium	The data are from a publicly available source without peer-review.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	ty Determi	ination	Medium	

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

Study Citation: OECD Harmonized	EC/HC, (2017). Water Solubility	Draft screening assessment: Phthalate s	ubstance groupin	g.
Template: HERO ID:	5353181			
			EXTRACTIO	N
Parameter		Data		
Water Solubility		20.3 mg/L		
CASRN and Test Material		84-69-5; diisobutyl phthalate		
Confidentiality, Type, and	Guideline	no; experimental; Not Reported		
Solvent, Reactivity, Storag		NR; NR; NR		
Radiolabel, Source, State,	•	NR; NR; NR; NR		
Temperature	Ž	not specified		
System		not specified		
рH		not specified		
Results Details Method		not specified		
Standard Deviation Results		not specified		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data 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 Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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.

Overall Quality Determination

Metric 5:

Metric 6:

Databases

Models

High

N/A

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.

Rating of this factor is not applicable to this kind of information.

^{*} Related References: Source cited: Haynes and Lide 2010

Diisobutyl Phthalate Water Solubility HERO ID: 679967 Table: 1 of 3

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

Template:

		EXTRACTIO	N
Parameter	Data		
Water Solubility	1E5 ug/L		
CASRN and Test Material	Not Reported; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	No; not specified; Not Reported		
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Temperature	20 deg C		
System	Not Reported		
рН	Not Reported		
Results Details Method	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	Not Reported		
		EVALUATIO	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Low	The present authors believe that value are wrong in the light of the other figures quoted.
Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other			
Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

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

Diisobutyl Phthalate Water Solubility HERO ID: 679967 Table: 2 of 3

Study Citation:

ECETOC, (1985). An assessment of the occurrence and effects of dialkyl ortho-phthalates in the environment.

OECD Harmonized

Water Solubility

Template: HERO ID:

HERO ID: 679967		DAMED A CONTON	
Parameter	Data	EXTRACTION	
Water Solubility	2E4 ug/L		
CASRN and Test Material	Not Reported; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	No; not specified; Not Reported		
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Repor	ted; Not Reported	
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Repor	ted; 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 Determine	ination	Modium	
Overall Quality Determine	ination	Medium	

^{*} Related References: Citing Leyder and Boulanger (1983) HERO ID 679764.

Diisobutyl Phthalate Water Solubility HERO ID: 679967 Table: 3 of 3

Study Citation:

ECETOC, (1985). An assessment of the occurrence and effects of dialkyl ortho-phthalates in the environment.

OECD Harmonized Template:

Water Solubility

Template: HERO ID:

		EXTRACTION	
Parameter	Data		
Water Solubility	6E3 ug/L		
CASRN and Test Material	Not Reported; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	No; not specified; Not Reported		
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported	ed; 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 Determ	ination	Medium	

^{*} Related References: Citing Hollifield, H.C. (1974). Rapid nephetometric estimate of water solubility of highly insoluble organic chemicals of environmental interest. Bull. Envir.Contam. Toxicol., 23, 579. no HERO ID.

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.

Reliability/Unbiased

(Method Objectivity)

Databases

Reliability/Analytical Method

Study Citation:

Domain 2: Test Reliability

Domain 3: Other

Metric 3:

Metric 4:

Metric 5:

OECD Harmonized	Water Solubilit	y	aces. Timexes.	
Template: HERO ID:	7325405			
			EXTRACTIO	N
Parameter		Data		
Water Solubility		20 mg/L		
CASRN and Test Material		84-69-5; Di-isobutyl phthalate		
Confidentiality, Type, and	Guideline	none; not specified; not specified		
Solvent, Reactivity, Storag	ge, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; liquid; NR		
Temperature		20°C		
System		not specified		
pH		not specified		
Results Details Method		not specified		
Standard Deviation Result	S	not specified		
Results Details		not specified		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.

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

Medium

Low

High

There is no indication that the methodology for producing the information was biased

The analytical method is unknown and there is no indication that a reliable method was

The information or data is from a recognized data collection/repository where data are

towards a particular product or outcome.

^{*} Related References: Source cited: Annex XV dossier (2009) Annex XV dossier (2009). Proposal for Identification of a Substance as SVHC (CMR), Diisobutyl phthalate, Submitted by Germany, August 2009. Available at: http://echa.europa.eu/doc/consultations/svhc/svhc_axvrep_germany_cmr_diisobutylphthalate_20090831.pdf

Diisobutyl Phthalate Water Solubility HERO ID: 5926421 Table: 1 of 1

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

Template:

TITTE	ACTION	

	EXTRACTION
Parameter	Data
Water Solubility	5.1 - 9.6 mg/L
CASRN and Test Material	84-69-5; Diisobutyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR
Temperature	25°C
System	Not Reported
pН	Not reported
Results Details Method	Reported as 0.0051 to 0.0096 g/L at 25 C
Standard Deviation Results	Not Reported
Results Details	2 data points were reported in Reaxys; 2 values were reported as 0.0051 to 0.0096 g/L at standard temperature.

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	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 Reliab	ility			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		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 Qual	ity Determ	ination	High	

^{*} Related References: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb. 4; (1997); p. 667 - 749

Diisobutyl Phthalate Water Solubility HERO ID: 7401366 Table: 1 of 1

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

Water Solubility

Template:

	EXTRACTION
Parameter	Data
Water Solubility	6.2 mg/L
CASRN and Test Material	Not Reported; diisobutyl phthalate
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	0.5% or less stock in ethanol or acetone. Adjusted with same solvent until 0.5 -1.5 mL standard produced turbid suspension in 40 mL water.; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; Liquid; NR
Temperature	$24\pm2^{\circ}\mathrm{C}$
System	Spectrophotofluorometer with a photomultiplier photometer, potted photomultiplier tube, and 150 W xenon arc lamp; test substance analyzed in standard 1-cm path length quartz fluorescence cuvette.
pН	Not reported
Results Details Method	Study performed at constant slit width, 3,2,2,3,5 slit arrangement. Excitation and emission monochromators set to 600 nm.
Standard Deviation Results	Not Reported
Results Details	40 mL water, 1 mL gum tragacanth solution (stock 0.10 g/L in water) used to prevent suspensions, and test substance added by syringe at 0.1 mL/min were stirred by magnetic stirrer until first signs of turbidity. This was repeated with 0.1 mL increasing quantities of test substance to create 6-8 standards. Turbid solutions allowed to rest for 15 min, resuspended by stirring, and nephelometric measurements were recorded. Calibration curve extrapolated to blank prepared without test substance to determine solubility.

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	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 Reliabi	ility			
	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.

^{*} 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).

Stud	v Citation:	Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water	partition
Diuu,	y Citation.	islak, 11., Stephan, 3., Karam, K., Codiadder, C., Wokoci, 1., Sanoa, C., Saao, 3. (2010). Addeous solubility, vapor pressure and octanor-water	partition

coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-

OECD Harmonized

Template:

370. Water Solubility

HERO ID: 3475635

	EXTRACTION				
Parameter	Data				
Water Solubility	7.080E-7				
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate				
Confidentiality, Type, and Guideline	None; Experimental; Not reported				
Solvent, Reactivity, Storage, and Stability	NR; NR; NR				
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.				
Temperature	298.15 K				
System	Water solubility measured using a dynamic saturation apparatus with quantification via HPLC-UV. Methanol was used as the solvent for elution.				
рН	Not reported				
Results Details Method	Temperature measurement accuracy was ± 0.02 K.				
Standard Deviation Results	2.54E-6				
Results Details	Value reported as mole fraction, where mole fraction = n solute / (n water + n solute). The value could not be converted to standard units as the volume of water used was not reported in this paper. Value initially reported as 7.080E7 but based on later references to solubilities of "10^-7", this is believed to be a typo. Average of three replicates measured at atmospheric pressure.				

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

Continued on next page ...

Diisobutyl Phthalate Water Solubility HERO ID: 3475635 Table: 1 of 5

... continued from previous page

Study Citation: Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition

coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-

OECD Harmonized

370. Water Solubility

Template:

		EVALUATION		
Domain	Metric	Rating	Comments	
Overall Quality Deter	mination	Medium		

Diisobutyl Phthalate Water Solubility HERO ID: 3475635 Table: 2 of 5

Study Citation: Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition

coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-

OECD Harmonized

370. Water Solubility

Template:

HERO ID: 3475635

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

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

Overall Quality Determination

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

OECD Harmonized

370. Water Solubility

OECD Harmonized Template: HERO ID:	Water Solubilit 3475635	у		
			EXTRACTION	
Parameter		Data		
Water Solubility		8.072E-7		
CASRN and Test Material 84-69-5; Di-iso-butyl phthalate				
Confidentiality, Type, and	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storag		NR; NR; NR		
Radiolabel, Source, State,		NR; Sigma-Aldrich; NR; 99% Notes: Use	d without further purif	ication.
Temperature	•	308.15 K	1	
System		Water solubility measured using a dynami	c saturation apparatus	with quantification via HPLC-UV. Methanol was used as the solvent for elution.
pН		Not reported		
Results Details Method		Temperature measurement accuracy was ±	Ε0.02 K.	
Standard Deviation Results	S	2.01E-1		
Results Details			this paper. Value initi	/ (n water + n solute). The value could not be converted to standard units as the ally reported as 8.072E7 but based on later references to solubilities of "10^-7", d at atmospheric pressure.
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance		_		
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Data cannot be converted to standard units and therefore appropriateness cannot be verified, but is likely to be appropriate based on the data's inclusion in a peer-reviewed article.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Study Citation: Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition

coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-

OECD Harmonized

370. Water Solubility

Template:

HEDU ID 3/75635

	EXTRACTION				
arameter	Data				
Vater Solubility	8.590E-7				
ASRN and Test Material	84-69-5; Di-iso-butyl phthalate				
onfidentiality, Type, and Guideline	None; Experimental; Not reported				
olvent, Reactivity, Storage, and Stability	NR; NR; NR				
adiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Used without further purification.				
emperature	313.15 K				
ystem	Water solubility measured using a dynamic saturation apparatus with quantification via HPLC-UV. Methanol was used as the solvent for elution.				
Н	Not reported				
esults Details Method	Temperature measurement accuracy was ± 0.02 K.				
tandard Deviation Results	4.20E-5				
esults Details	Value reported as mole fraction, where mole fraction = n solute / (n water + n solute). The value could not be converted to standard units as the volume of water used was not reported in this paper. Value initially reported as 8.590E7 but based on later references to solubilities of "10^-7", this is believed to be a typo. Average of three replicates measured at atmospheric pressure.				

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

Overall Quality Determination

Study Citation: Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition

coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-

OECD Harmonized

370. Water Solubility

Tompletee

		EXTRACTION		
Parameter	Data			
Water Solubility	11.254E-7			
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes	: Used without further purif	fication.	
Temperature	323.15 K			
System Water solubility measured using a dynamic saturation apparatus with quantification via HPLC-UV. Methanol was used as the solvent for			with quantification via HPLC-UV. Methanol was used as the solvent for elution.	
pH Not reported				
Results Details Method	Temperature measurement accuracy was ± 0.02 K.			
Standard Deviation Results	1.57E-6			
Results Details		ed in this paper. Value initi	/ (n water + n solute). The value could not be converted to standard units as the ally reported as 11.254E7 but based on later references to solubilities of "10^-7", d at atmospheric pressure.	
		EVALUATION		
Domain	Metric	Rating	Comments	
Domain 1: Substance				
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.	
Metric 2:	Appropriateness	Medium	Data cannot be converted to standard units and therefore appropriateness cannot be verified, but is likely to be appropriate based on the data's inclusion in a peer-revie	

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

Overall Quality Determination

Water Solubility Diisobutyl Phthalate HERO ID: 807140 Table: 1 of 1

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. Water Solubility

OECD Harmonized

Template:

HERO ID: 807140

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

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabi	ility			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
		(Method Objectivity)		
	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 unac ceptable.

Overall Quality Determination

NLM, (2013). PubChem: Hazardous Substance Data Bank: Diisobutyl phthalate, 84-69-5.

Study Citation:

OECD Harmonized Water Solubility Template: **HERO ID:** 5926117 **EXTRACTION** Data **Parameter** Water Solubility 6.2 mg/L CASRN and Test Material 84-69-5; Diisobutyl phthalate Confidentiality, Type, and Guideline None; Experimental; Not reported Solvent, Reactivity, Storage, and Stability NR; NR; NR; NR Radiolabel, Source, State, and Purity Not Reported; NR; NR; NR Temperature 24°C System Not Reported pН Not reported Results Details Method Not Reported Standard Deviation Results Not Reported Results Details Not Reported

			EVALUATIO:	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	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 Reliab	ility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Qual	Overall Quality Determination			

^{*} Related References: Yalkowsky, S.H., He Yan, Jain, P. Handbook of Aqueous Solubility Data Second Edition. CRC Press, Boca Raton, FL 2010. p. 1111

Study Citation:	U
OECD Harmonized	W

U.S. EPA, (2019). Chemistry Dashboard Information for Diisobutyl phthalate. 84-69-5..

Water Solubility

Template:

		EXTRACTIO	N
Parameter	Data		
Water Solubility	6.2 mg/L		
CASRN and Test Material	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR		
Temperature	Not Reported		
System	Not Reported		
pН	Not reported		
Results Details Method	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	Unit conversion conducted to obtain 6.2	mg/L. Reported as	2.23e-5 mol/L.
		EVALUATIO	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	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 Determ	ination	High	

^{*} Related References: PhysProp. Yalkowsky, SH and DannenFelser, RM (1992)

Diisobutyl Phthalate Flash Point HERO ID: 5155508 Table: 1 of 1

Study Citation: OECD Harmonized	CPSC, (2015). Exposure assessment: Composition, production, and use of phthalates. Flash Point			
Template:				
HERO ID:	5155508			
			EXTRACTION	
Parameter		Data		
Flash Point		161 - 185 C		
CASRN and Test Material		84-69-5; di-isobutyl phthalate		
Confidentiality, Type, and	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; liquid; NR		
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	The data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)	_	towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data is from a publicly available secondary source without peer-review.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	Medium	

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

Diisobutyl Phthalate Flash Point HERO ID: 6629592 Table: 1 of 2

Study Citation: OECD Harmonized	NCBI, (2020). PubChem Compound Summary for CID 6782 Diisobutyl phthalate. flash Point			late.
Template:	((20502			
HERO ID:	6629592			
D 4		D 4	EXTRACTION	
Parameter		Data		
Flash Point		385 F		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; not specified; Not reported		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
System		Not reported		
Standard Deviation Result	S	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 Reliabi	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	Metric 4:	(Method Objectivity) Reliability/Analytical Method	Low	towards a particular product or outcome. The analytical method is unknown and there is no indication that a reliable method was
	Meure 4.	Remadificy/Analytical Method	Low	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 Quali	tv Dotormi		Medium	
Over an Quan	y Determi	เมลมงม	Miculain	

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

Diisobutyl Phthalate Flash Point HERO ID: 6629592 Table: 2 of 2

Study Citation:	
OTION II	_

NCBI, (2020). PubChem Compound Summary for CID 6782 Diisobutyl phthalate.

OECD Harmonized

Flash Point

Template:

ID: 6629592

		EXTRACTION	
Parameter	Data		
Flash Point	365 F		
CASRN and Test Material	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	None; not specified; Not reported		
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, and Purity	NR; NR; NR; NR		
System	Open cup		
Standard Deviation Results	Not reported		
Results Details	185°C		
		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.

Overall Quality Determination

Metric 5:

Metric 6:

Medium

Medium

N/A

Data is from a secondary database with a reference to the original source.

Rating of this factor is not applicable to this kind of information.

Databases

Models

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

Study Citation: OECD Harmonized	NLM, (2013). P Flash Point	PubChem: Hazardous Substance Data E	Bank: Diisobutyl pl	nthalate, 84-69-5.
Template:				
HERO ID:	5926117			
			EXTRACTIO	N
Parameter		Data		
Flash Point		365 F		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
System		Open cup		
Standard Deviation Results	S	Not reported		
Results Details		185°C		
			EVALUATIO	N
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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	High	

^{*} Related References: National Fire Protection Association; Fire Protection Guide to Hazardous Materials. 14TH Edition, Quincy, MA 2010, p. 325-47

Study Citation: OECD Harmonized	RSC, (2019). C Flash Point	ChemSpider: Diisobutyl phthalate.		
Template:				
HERO ID:	5926262			
			EXTRACTION	
Parameter		Data		
Flash Point		169 C		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage		NR; NR; NR		
Radiolabel, Source, State,		Not Reported; NR; NR; NR		
System	•	Not Reported		
Standard Deviation Results	3	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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Quali	ty Determi	ination	Medium	

^{*} Related References: Alfa Aesar

Study Citation: OECD Harmonized	RSC, (2019). C Flash Point	hemSpider: Diisobutyl phthalate.		
Template:				
HERO ID:	5926262			
			EXTRACTION	
Parameter		Data		
Flash Point		336.2 F		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and C		None; Experimental; Not reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	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.
D : 0 T (D ! 1 ! 1 !	•.			
Domain 2: Test Reliabil	•	D 1: 1:1:4 /II 1: 1	3.6.11	
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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.
D : 2 O.1				
Domain 3: Other	Matria 5.	Databases	Madin	Date in from a million and the land and an arranged and arranged arranged and arranged and arranged arranged and arranged arra
	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

^{*} Related References: Alfa Aesar

Diisobutyl Phthalate Flash Point HERO ID: 5926262 Table: 3 of 3

Study Citation: OECD Harmonized Template:	RSC, (2019). Cl Flash Point	hemSpider: Diisobutyl phthalate.		
HERO ID:	5926262			
			EXTRACTION	
Parameter		Data		
Flash Point		180 C		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	Not Reported; NR; NR; NR		
System		Not Reported		
Standard Deviation Results	S	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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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.

Overall Quality Determination

Metric 5:

Metric 6:

Databases

Models

Domain 3: Other

Medium

N/A

Medium

Data is from a publicly available secondary source with references to non-peer reviewed

Rating of this factor is not applicable to this kind of information.

^{*} Related References: LabNetwork

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

OECD Harmonized	Flash Point			
Template: HERO ID:	6655446			
HERO ID:	0033440			
Parameter		Data	EXTRACTIO	N
r ai ainetei		Data		
Flash Point		185 C		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storag	ge, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	Not Reported; NR; NR; NR		
System		Not reported		
Standard Deviation Result	S	Not reported		
Results Details		Not Reported		
- ·			EVALUATIO	
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 Reliabi	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a known data-collection, prepared by experts in the field.
	Michie J.		J	/ I I / I

Overall Quality Determination

High

Study Citation: OECD Harmonized Template:	farmonized Autoflammability			nthalate, 84-69-5.
HERO ID:	5926117			
			EXTRACTIO	N
Parameter		Data		
Auto-flammability		810 F		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and C	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	and Purity	NR; NR; NR; NR		
System		Not reported		
Standard Deviation Results	;	Not reported		
Results Details		432°C		
Results Value		Not Reported		
			EVALUATIO	N
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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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.

^{*} Related References: National Fire Protection Association; Fire Protection Guide to Hazardous Materials. 14TH Edition, Quincy, MA 2010, p. 325-47

Overall Quality Determination

High

Study Citation: OECD Harmonized Sigma-Aldrich, (2020). Diisobutyl phthalate safety data sheet.

Autoflammability

Template:

DXZDD	ACTION	
HXIR	ACTION	

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

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance	;			
	Metric 1:	Representativeness	High	Data is reported for the target chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Relia	bility			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other			_	
	Metric 5:	Databases	Low	Data is from a known chemical supplier. The data are from a primary source without expert peer-review or an unknown secondary source without peer-review and references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qua	lity Determ	ination	Low	

Study Citation: OECD Harmonized Template:	NLM, (2013). Viscosity	PubChem: Hazardous Substance Data Ba	ank: Diisobutyl pl	nthalate, 84-69-5.
HERO ID:	5926117			
			EXTRACTIO	N
Parameter		Data		
Viscosity		41		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage		NR; NR; NR		
Radiolabel, Source, State, a	-	Not Reported; NR; NR; NR		
Temperature	-	20°C		
Test Conditions		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		41 mPa.S		
			EVALUATIO	N
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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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				
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 Qualit	ty Determi	nation	High	

^{*} Related References: Gerhartz, W. (exec Ed.) Ullmann's Encyclopedia of Industrial Chemistry. 5th Ed. Vol A1: Deerfield Beach, FL: VCH Publishers. p. VA20 193.

EXTRACTION

Diisobutyl Phthalate Refractive Index HERO ID: 5926421 Table: 1 of 1

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

Template:

Parameter	Data		
Refractive Index	1.491		
CASRN and Test Material	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, and Purity	Not Reported; NR; NR; NR		
Temperature	20°C		
System	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	Not Reported		
Results Details Methods	Not Reported		
Parameter	Wavelength: 589 nm		
		EVALUATIO	N
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	Medium	There is no indication that the methodology for producing the information was biased
	(Method Objectivity)		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 Determi	nation	High	

^{*} Related References: Fischer et al.; Pharmazeutische Zentralhalle; vol. 105; (1966); p. 73,74,

Diisobutyl Phthalate Refractive Index HERO ID: 5926117 Table: 1 of 1

Study Citation: NLM, (2013). PubChem: OECD Harmonized Refractive Index

 $NLM, (2013). \ Pub Chem: \ Hazardous \ Substance \ Data \ Bank: \ Diisobutyl \ phthalate, 84-69-5.$

Template:

		EXTRACTIO	N
Parameter	Data		•
Refractive Index	1.4900		
CASRN and Test Material	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage, and Stability	NR; NR; NR		
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		
		EVALUATIO	
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 Determi	nation	High	

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

Diisobutyl Phthalate Refractive Index HERO ID: 5926262 Table: 1 of 1

Study Citation: OECD Harmonized	RSC, (2019). C Refractive Inde	ChemSpider: Diisobutyl phthalate.		
Template: HERO ID:	5926262			
			EXTRACTION	
Parameter		Data		
Refractive Index		1.49		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storag		NR; NR; NR		
Radiolabel, Source, State,	·	Not Reported; NR; NR; NR		
Temperature	•	Not Reported		
System		Not Reported		
Standard Deviation Results	S	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 Reliabil	litv			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		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

^{*} 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. Henry's Law

OECD Harmonized

Template:

HERO ID: 4159647

TIXZED		TANT
EXTR	ΑCI	TON

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

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 Reliab	oility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6:	Models	High	The model had a defined, unambiguous endpoint AND the model performance was known and $r2 > 0.7$, $q2 > 0.5$, and $SE < 0.3$.

Overall Quality Determination High

Study Citation: Elsevier, (2019). Reaxys: physical-chemical property data for diisobutyl phthalate. CAS Registry Number: 84-69-5 Henry's Law Template:			ohthalate. CAS Registry Number: 84-69-5	
HERO ID:	5926421			
			EXTRACTIO	N
Parameter		Data		
Henry's Law		1.83E-7 atm-m3/mol		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	and Purity	Not Reported; NR; NR; NR		
Temperature		Not reported		
pН		Not Reported		
System		Not Reported		
Standard Deviation Results	\$	Not Reported		
Results Details		Not Reported		
Results Details Methods		Not Reported		
			EVALUATION	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		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 Qualit	ty Determi	nation	High	

^{*} Related References: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb.4; (1997); p. 667 - 749

Ct.,d	Citation	ak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partit	tion
Study	Citation:	ak, n., Stephan, J., Karam, K., Goutaudiei, C., Mokdei, I., Sanda, C., Saad, J. (2010). Aquedus soludinty, vapor pressure and octanor-water partit	11011

coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-

370. Henry's Law

OECD Harmonized

Template:

EXTR	$\Delta C'$	TION	J

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

		EVALUATION				
Domain		Metric	Rating	Comments		
Domain 1: Substance						
M	letric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.		
М	Ietric 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						
M	letric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.		
М	letric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate, based on methods used to derive calculation inputs.		
Domain 3: Other						
M	letric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.		
M	letric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.		

Study Citation: Ishak, H., Stephan, J., Karam, R., Goutaudier, C., Mokbel, I., Saliba, C., Saab, J. (2016). Aqueous solubility, vapor pressure and octanol-water partition

coefficient of two phthalate isomers dibutyl phthalate and di-isobutyl phthalate contaminants of recycled food packages. Fluid Phase Equilibria 427:362-

OECD Harmonized

370. Henry's Law

Tompletee

Template:			
HERO ID: 3475635			
		EXTRACTIO	N
Parameter	Data		
Henry's Law	10.77 Pa⋅m3/J		
CASRN and Test Material	84-69-5; Di-iso-butyl phthalate		
Confidentiality, Type, and Guideline	None; Calculation; Non-guideline		
Solvent, Reactivity, Storage, and Stabil	ity NR; NR; NR		
Radiolabel, Source, State, and Purity	NR; Sigma-Aldrich; NR; 99% Notes: Us	sed without further	purification.
Temperature 298.15 K			
pH	Not reported		
System			r's law constant based on experimental vapor pressure (0.0105 Pa) and mole fraction of
water solubility (7.080 x 10^-7); WS: dynamic saturation method; VP: dynamic gas saturation method			nethod; VP: dynamic gas saturation method
Standard Deviation Results Not reported			
Results Details		-	ary's law constant; Mw: molar mass, R: gas constant, ρ w: density of water)
Results Details Methods	experimental vapor pressure: HPLC-UV	and water solubili	ty: HPLC-UV (using an internal calibration method with BBP)
		EVALUATIO	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1	: Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2	: Appropriateness	High	Measured data are consistent with the subject chemical substance structural features
			(e.g., presence of certain functional groups) [and/or] other physical/chemical properties.
D			
Domain 2: Test Reliability	D 1: 1:1: /// 1	3.6.12	
Metric 3	3	Medium	There is no indication that the methodology for producing the information was biased
3.5	(Method Objectivity)	TT: _1	towards a particular product or outcome.
Metric 4	: Reliability/Analytical Method	High	The analytical methods are appropriate.
Domain 3: Other			
Metric 5	: Databases	High	The information or data is from a recognized data collection/repository where data are
Wette 5			peer-reviewed by experts in the field, are broadly available to the public for review and
			use OR includes references to the original sources.

Overall Quality Determination

Metric 6:

Models

High

N/A

Rating of this factor is not applicable to this kind of information.

Diisobutyl Phthalate Henry's Law HERO ID: 807140 Table: 1 of 1

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.

Not Reported

OECD Harmonized

Results Details Methods

Henry's Law

Template:

HERO ID: 807140

EXTRACTION		
	Parameter	Data
	Henry's Law	Not Reported
	CASRN and Test Material	84-69-5; diisobutyl phthalate
	Confidentiality, Type, and Guideline	none; QSAR; Quantitative Structure-Property relationship model for estimation of log Kaw
	Solvent, Reactivity, Storage, and Stability	NR; NR; NR
	Radiolabel, Source, State, and Purity	NR; NR; NR Notes: DIBP
	Temperature	Not Reported
	pH	Not Reported
	System	Kaw = S(A)/Sw where $S(A)$ is the solubility in air and Sw is the solubility in water
	Standard Deviation Results	Not Reported
	Results Details	Log Kaw= -4.30

			EVALUATION	
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 Reliab	oility			
	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

Study Citation:	
OECD Harmonized	ł

U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).

Henry's Law

Metric 5:

Metric 6:

Template:

		EXTRACTION	
Parameter	Data		
Henry's Law	6.43E-7 - atm-m^3/mole		
CASRN and Test Material	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	No; not specified; NR		
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reporte	d; Not Reported	
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reporte		
Temperature	NR		
pH	NR		
System	Not Reported		
Standard Deviation Results	NR		
Results Details	NR		
Results Details Methods	NR		
		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.

Medium **Overall Quality Determination**

Models

Databases

Medium

N/A

original sources.

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

Rating of this factor is not applicable to this kind of information.

^{*} Related References: Cites secondary source: NICNAS (National Industrial Chemicals Notification and Assessment Scheme). (2008) Diisobutyl phthalate. Existing chemical hazard assessment report. Australian Government. Available online athttp://www.nicnas.gov.au/Publications/CAR/Other/DiBPP%20hazard%20assessment.pdf (accessed October 13, 2010). HEROID 2316625

Diisobutyl Phthalate Henry's Law HERO ID: 5155528 Table: 2 of 2

Study Citation:

U.S. Consumer Product Safety Commission (CPSC) (2011). Toxicity review of diisobutyl phthalate (DiBP, CASRN 84-69-5).

OECD Harmonized

Henry's Law

Template:

HERO ID: 5155528			
D	D 4	EXTRACTION	
Parameter	Data		
Henry's Law	1.22E-06 - atm-m^3/mole		
CASRN and Test Material	84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and Guideline	No; not specified; NR		
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported	ed: Not Reported	
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported		
Temperature	25 deg C	. 1	
pH	NR		
System	Not Reported		
Standard Deviation Results	NR		
Results Details	NR		
Results Details Methods	NR		
		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Substance	1,101110	- Tuning	
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features
	II II		(e.g., presence of certain functional groups) or other physical/chemical properties.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other			
Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Orranall Orrallar D.4	: a4: a	Madie	
Overall Quality Determ	เเกลนอก	Medium	

^{*} Related References: Cites secondary source: HSDB (Hazardous Substance Data Bank). (2009) Diisobutyl phthalate. National Library of Medicine HSDB Database. (Last Revision, 01/05/2009). Same source but previous version of HEROID 5926117. Not previously extracted, HEROID in distiller.

HERO ID: 5926421 Table: 1 of 1

Diisobutyl Phthalate Dielectric Constant

Study Citation: OECD Harmonized	Elsevier, (2019) Dielectric Cons		ta for diisobutyl _l	phthalate. CAS Registry Number: 84-69-5
Template: HERO ID:	5926421			
			EXTRACTIO	N
Parameter		Data		
CASRN and Test Material		84-69-5; Diisobutyl phthalate		
Confidentiality, Type, and C	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage	, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	nd Purity	Not Reported; NR; NR; NR		
Dielectric Constant		6.56		
Temperature		25°C		
System		Not Reported		
Results Value		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
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 Reliabili	ty			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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 Qualit	v Determi	nation	High	

^{*} Related References: Buchner; Barthel; Berichte der Bunsengesellschaft/Physical Chemistry Chemical Physics;vol. 101; nb. 10; (1997); p. 1509 - 1516

Diisobutyl Phthalate Other Properties HERO ID: 807140 Table: 1 of 1

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

EVTD	ACT	TION
EXTR	Aι	HUN

CASRN and Test Material
Confidentiality, Type, and Guideline
Solvent, Reactivity, Storage, and Stability
Radiolabel, Source, State, and Purity

Data

84-69-5; diisobutyl phthalate
none; QSAR; Quantitative Structure-Property relationship model for estimation of log Koa
NR; NR; NR; NR
NR; NR Notes: DIBP

Results Value Log Koa = 8.38

Results Details Koa = So/S(A) where So is solubility in octanol and S(A) is the solubility in air

Results Remarks Not Reported

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliab	oility			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
		(Method Objectivity)		
	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

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List of Abbreviations and Acronyms for Data Quality Evaluation and Extraction Tables

Term	Definition			
ASTM	American Society for Testing and Materials			
ATSDR	Agency for Toxic Substances and Disease Registry			
atm	Atmospheres			
atm · m ³ /mol	Atmospheres - cubic meters per mole			
C	Celsius			
CASRN	Chemical Abstract Service registry number			
cP	Centipoise			
CRC	CRC Handbook of Chemistry and Physics			
DOE	U.S. Department of Energy			
ECB	European Chemicals Bureau			
EPA	Environmental Protection Agency			
F	Fahrenheit			
GC	Gas Chromatography			
g/cm ³	Grams per cubic centimeter			
GLP	Good Laboratory Practice			
HLC	Henry's Law Constant			
HPV	High Production Volume			
HSDB	Hazard Substance Data Bank			
ILO	International Labour Organization			
IPCS	International Programme on Chemical Safety			
IUCLID	International Uniform Chemical Information Database			
K	Kelvin			
Koa	Octanol-Air partition coefficient			
Kow	Octanol-Water partition coefficient			
mg/L	Milligrams per Liter			
mol	Mole			
mmHg	Millimeters of Mercury			
MS	Mass Spectrometry			
N/A	Not Applicable			
NICNAS	National Industrial Chemicals Notification and Assessment Scheme			
NLM	National Library of Medicine			
NR	Not Reported			
OECD	Organisation for Economic Co-operation and Development			
Pa (hPa)	Pascals (hectopascals; 1 hPa = 100 Pa)			
pН	Negative base 10 Log of Hydrogen Ion (H+) Concentration in Aque-			
	ous Solution			
pKa	Negative base 10 Log of Acid Dissociation Constant (Ka)			
RIVM	National Institute for Public Health and the Environment (Dutch: Ri-			
	jksinstituut voor Volksgezondheid en Milieu)			
	Continued on next nego			

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... continued from previous page

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