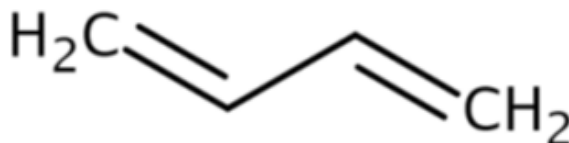

**Data Quality Evaluation and Data Extraction Information for
Physical and Chemical Properties for
1,3-Butadiene**

Systematic Review Support Document for the Risk Evaluation

CASRN: 106-99-0



December 2025

This supplemental file contains information regarding the data extraction and evaluation results for data sources that were considered for the *Risk Evaluation for 1,3-Butadiene* 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 *Risk Evaluation for 1,3-Butadiene – Systematic Review Protocol*. 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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5349218	Sun, H. N., Wristers, J. P. (2002). Butadiene.	220
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Study Citation:	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.			
OECD Harmonized Template:	Physical Form or State			
HERO ID:	5155603			
EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Results Value	Colorless gas			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: No source cited; extracted gray lit

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.			
OECD Harmonized Template:	Physical Form or State			
HERO ID:	3981013			
EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	none; not specified; not specified			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Results Value	gas			
Results Details	not specified			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5160048

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; colorless gas at 25 C with a mild aromatic odor; Not Reported
Results Value	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from Mackay, D., W.Y. Shiu and K.C. Ma. 1993. Illustrated handbook of physical-chemical properties and environmental fate of organic compounds. Vol. III. Lewis Publishers Inc., Chelsea, Michigan

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5155560

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; colorless gas with a mild aromatic odor.; Not Reported
Results Value	Not Reported
Results Details	reported at n.t.p; The odour threshold limit is between 1.0 and 4.0 mg/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 Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

High

* Related References: missing reference

Study Citation:	Haz-Map (n.d.). Hazardous agents: 1,3-Butadiene.			
OECD Harmonized Template:	Physical Form or State			
HERO ID:	7681901			
EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	none; not specified; not specified			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; gas; NR			
Results Value	Colorless gas with a mild aromatic or gasoline-like odor			
Results Details	liquid below 24°F as a compressed gas			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are reported for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. Secondary source citing secondary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Citation: HSDB - HERO ID 6628926 (not in distiller PChem at time of extraction)

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.
OECD Harmonized Template:	Physical Form or State
HERO ID:	9493542

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; highly reactive, colorless gas with a mildly aromatic odor; Not Reported
Results Value	Not Reported
Results Details	Not Reported

EVALUATION

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

Overall Quality Determination**High**

* Related References: cited from M. Windholz, ed., The Merck Index, 10th ed., Merck & Co., Inc., Rahway, NJ, 1983,p. 1480.

Study Citation:	National Toxicology Program (NTP), (1993). NTP technical report on the toxicology and carcinogenesis studies of 1,3-butadiene (CAS no. 106-99-0) in B6C3F1 mice (inhalation studies).
OECD Harmonized Template:	Physical Form or State
HERO ID:	5160111

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; colorless, noncorrosive gas; Not Reported
Results Value	Not Reported
Results Details	Kirshenbaum, 1978

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

Overall Quality Determination

High

* Related References: Citing from Kirshenbaum, I. (1978). Butadiene. In Kirk-Othmer Encyclopedia of Chemical Technology, Vol. 4, 3rd ed., pp. 313-337. John Wiley and Sons, New York.

Study Citation:	National Toxicology Program (NTP), (2016). Report on carcinogens, fifteenth edition: 1,3-butadiene.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5160138

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; colorless gas with a mild aromatic or gasoline odor at room temperature; Not Reported
Results Value	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: no references cited

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.
OECD Harmonized Template:	Physical Form or State
HERO ID:	10171483

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported Notes: Mild aromatic odor
Results Value	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 267 (HERO ID: 5926379)

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.			
OECD Harmonized Template:	Physical Form or State			
HERO ID:	192177			
EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; Gas; NR Notes: NR			
Results Value	Colorless gas; mild aromatic or gasoline-like odor			
Results Details	liquid at <24°F; shipped as a liquefied compressed gas			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	NIOSH, (1992). Occupational safety and health guideline for butadiene (1,3-butadiene).			
OECD Harmonized Template:	Physical Form or State			
HERO ID:	8408503			
EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; Not Reported			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; shipped under its own vapor pressure as a liquified gas; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; colorless, flammable gas with a mild aromatic odor. The odor threshold is reported to be 1.1 parts per million parts of air; Not Reported			
Results Value	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: no references cited

Study Citation:	Sun, H. N., Wristers, J. P. (2002). Butadiene.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5349218

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; noncorrosive, colorless, flammable gas at room temperature and atmospheric pressure with a mildly aromatic odor; Not Reported
Results Value	Not Reported
Results Details	Not Reported

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

Overall Quality Determination	Medium
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* Related References: no references cited

Study Citation:	U.S. EPA, (1985). Mutagenicity and carcinogenicity assessment of 1,3-butadiene. Review draft.
OECD Harmonized Template:	Physical Form or State
HERO ID:	10293377

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Value	colorless gas with a slight aromatic odor at room temperature and pressure
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: no references cited

Study Citation:	U.S. EPA, (1985). Mutagenicity and carcinogenicity assessment of 1,3-butadiene: Final report.
OECD Harmonized Template:	Physical Form or State
HERO ID:	1565

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, and Guideline	None; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; NR; NR
Results Value	colorless gas
Results Details	Not Reported

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

Overall Quality Determination	High
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Study Citation:	U.S. EPA, (2002). Health assessment of 1,3-butadiene.			
OECD Harmonized Template:	Physical Form or State			
HERO ID:	52153			
EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	none; not specified; NA			
Solvent, Reactivity, Storage, and Stability	NA; NA; NA; NA			
Radiolabel, Source, State, and Purity	NA; NA; gas; NA			
Results Value	colorless gas with mildly aromatic odor			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other	Metric 5:	Databases	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: Secondary source referencing: Sax, NI; Lewis, RJ, Sr. (1987) Hawley's condensed chemical dictionary, 11th ed. New York, NY: Van Nostrand Reinhold, p. 177.

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926134

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Value	gas
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: NIOSH Pocket Guide to Chemical Hazards. Department of Health and Human Services, Centers for Disease Control & Prevention. National Institute for Occupational Safety & Health. DHHS (NIOSH) 2010 (2010).

Study Citation:	O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926379

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Value	colorless gas
Results Details	Not Reported

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

Overall Quality Determination

High

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Physical Form or State			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Value	gas or pressurized liquid			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other	Metric 5:	Databases	Medium	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		High		

* Related References: Oxford University Chemical Safety Data

Study Citation:	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5349186

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Value	colorless gas
Results Details	Not Reported

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

Overall Quality Determination

High

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.
OECD Harmonized Template:	Physical Form or State
HERO ID:	5926134

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details	colorless, mildly aromatic or gasoline-like odor

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

Overall Quality Determination

High

* Related References: NIOSH Pocket Guide to Chemical Hazards. Department of Health and Human Services, Centers for Disease Control & Prevention. National Institute for Occupational Safety & Health. DHHS (NIOSH) 2010 (2010).

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Physical Form or State			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Details	colorless, odor TLV 1.6 ppm			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Oxford University Chemical Safety Data

Study Citation:	California Office of Environmental Health Hazard Assessment (OEHHA) (2011). Appendix B: Chemical-specific summaries of the information used to derive unit risk and cancer potency values.			
OECD Harmonized Template:	Melting Point			
HERO ID:	5155632			
EXTRACTION				
Parameter	Data			
Melting Point	-108.9 °C			
CASRN and Test Material	106-99-0; 1,3-BUTADIENE			
Confidentiality, Type, and Guideline	none; not specified; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Results Details Methods	NR			
Standard Deviation Results	NR			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Citing HSDB, 1998.

Study Citation:	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.			
OECD Harmonized Template:	Melting Point			
HERO ID:	5155603			
EXTRACTION				
Parameter	Data			
Melting Point	-108.9 °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Results Details Methods	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: No source cited; extracted gray lit

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.			
OECD Harmonized Template:	Melting Point			
HERO ID:	3981013			
EXTRACTION				
Parameter	Data			
Melting Point	-108.91 - °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	none; not specified; none			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Results Details Methods	not reported			
Standard Deviation Results	not reported			
Results Details	not reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.
OECD Harmonized Template:	Melting Point
HERO ID:	5160048

EXTRACTION	
Parameter	Data
Melting Point	-108.9 - °C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from Weast, R.C. (ed.). 1984. Handbook of Chemistry and Physics. 65th ed. CRC Press, Boca Raton, Florida

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for 1,3-butadiene. CAS Registry Number: 106-99-0..			
OECD Harmonized Template:	Melting Point			
HERO ID:	5926412			
EXTRACTION				
Parameter	Data			
Melting Point	-108.97 - -108.7 °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Details Methods	Measured conditions were not reported; 5 values were reported in Reaxys; 5 of these values were reported in the range of -108.97 to -108.7°C; 0 data points were outside the range.			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a secondary database with a references to the peer-reviewed original source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.
OECD Harmonized Template:	Melting Point
HERO ID:	9493526

EXTRACTION	
Parameter	Data
Melting Point	Not Reported
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Enthalpy of melting: 7.988 kJ/mol at 164.2 K, 101.3 kPa

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

Overall Quality Determination

High

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.
OECD Harmonized Template:	Melting Point
HERO ID:	9493542

EXTRACTION	
Parameter	Data
Melting Point	-108.915 - °C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Reported as freezing point in air at 101.3 kPa

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

Overall Quality Determination

High

* Related References: cited from F. O. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953.

Study Citation:	National Toxicology Program (NTP), (1999). NTP report on carcinogens background document for 1,3-butadiene.
OECD Harmonized Template:	Melting Point
HERO ID:	5160135

EXTRACTION	
Parameter	Data
Melting Point	-108.97 - °C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from Budavari, S., Ed. 1996. The Merck Index, 12th ed. Merck & Co, Inc., Whitehall, NJ.(HERO ID 670297)

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.
OECD Harmonized Template:	Melting Point
HERO ID:	10171483

EXTRACTION	
Parameter	Data
Melting Point	Not Reported
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Enthalpy of fusion: 7.98 kJ/mol

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

Overall Quality Determination

High

* Related References: Cited from Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-76 (HERO ID: 2828348)

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

EXTRACTION	
Parameter	Data
Melting Point	-164 - F
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Results Details Methods	NR
Standard Deviation Results	NR
Results Details	Reported as freezing point

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

Overall Quality Determination

High

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Melting Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Melting Point	164.5 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Results Details Methods	Not Reported			
Standard Deviation Results	0.2 K			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Kistiakowsky, G.B.; Ruhoff, J.R.; Smith, H.A.; Vaughan, W.E., Heats of Organic Reactions IV. Hydrogenation of Some Dienes and of Benzene, J. Am. Chem. Soc., 1936, 58, 146-53.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Melting Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Melting Point	164.210 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Results Details Methods	Not Reported			
Standard Deviation Results	0.04 K			
Results Details	Also report 164.210 K with standard deviation of 0.03 K in same chart under melting point.			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Streiff, A.J.; Soule, L.F.; Kennedy, C.M.; Janes, M.E.; Sedlak, V.A.; Willingham, C.B.; Rossini, F.D., Purification, purity, and freezing points of twenty-nine hydrocarbons of the API-standard and API-NBS series., J. Res. Natl. Bur. Stand. (U. S.), 1950, 45, 173.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Melting Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Melting Point	164.3 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Results Details Methods	Not Reported			
Standard Deviation Results	0.4 K			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Anonymous, R., , Am. Pet. Inst. Res. Proj. 45, Ohio State Univ., 1958.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Melting Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Melting Point	164.220 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Results Details Methods	Not Reported			
Standard Deviation Results	0.04 K			
Results Details	Also report 164.230 K with standard deviation of 0.02 K in same chart under melting point.			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Glasgow, A.R.; Krouskop, N.C.; Beadle, J.; Axilrod, G.D.; Rossini, F.D., Compounds involved in production of synthetic rubber. determination of purity by measurement of freezing points., Anal. Chem., 1948, 20, 410.

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.
OECD Harmonized Template:	Melting Point
HERO ID:	5926134

EXTRACTION	
Parameter	Data
Melting Point	-108.966 °C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

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

Study Citation:	O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.
OECD Harmonized Template:	Melting Point
HERO ID:	5926379

EXTRACTION	
Parameter	Data
Melting Point	-108.966 °C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

Study Citation:	O’Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.			
OECD Harmonized Template:	Melting Point			
HERO ID:	5926379			
EXTRACTION				
Parameter	Data			
Melting Point	-108.902 °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Details Methods	Freezing point			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Melting Point			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Melting Point	-108.9 °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Details Methods	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

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

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Melting Point			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Melting Point	-109 °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Details Methods	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Parchem-fine & specialty chemicals

Study Citation:	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.
OECD Harmonized Template:	Melting Point
HERO ID:	5349186

EXTRACTION	
Parameter	Data
Melting Point	-108.9 °C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..
OECD Harmonized Template:	Melting Point
HERO ID:	5926160

EXTRACTION	
Parameter	Data
Melting Point	-109 °C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 1,3-Butadiene. 106-99-0..			
OECD Harmonized Template:	Melting Point			
HERO ID:	5926160			
EXTRACTION				
Parameter	Data			
Melting Point	-109 °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Details Methods	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a publicly available database that references a peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: NIOSH

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..			
OECD Harmonized Template:	Melting Point			
HERO ID:	5926160			
EXTRACTION				
Parameter	Data			
Melting Point	-113 °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Details Methods	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

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

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..			
OECD Harmonized Template:	Melting Point			
HERO ID:	5926160			
EXTRACTION				
Parameter	Data			
Melting Point	-109 °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Details Methods	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

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

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..			
OECD Harmonized Template:	Melting Point			
HERO ID:	5926160			
EXTRACTION				
Parameter	Data			
Melting Point	-109 °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Details Methods	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: SynQuest

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..			
OECD Harmonized Template:	Melting Point			
HERO ID:	5926160			
EXTRACTION				
Parameter	Data			
Melting Point	-109 °C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Results Details Methods	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination			Medium	

* Related References: SynQuest

Study Citation:	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.
OECD Harmonized Template:	Melting Point
HERO ID:	6389860

EXTRACTION	
Parameter	Data
Melting Point	Not Reported
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Results Details Methods	Not Reported
Standard Deviation Results	Not Reported
Results Details	Heat of fusion 147.6 J/g (35.28 cal/g)

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

Overall Quality Determination

High

* Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed, Volume 4. New York, New York: John Wiley and Sons, 1978. (HERO ID 594584) and Hawley, G.G. 1,3-Butadiene. In: The Condensed Chemical Dictionary, 10th ed., New York, New York: Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID 69425)

Study Citation:	California Office of Environmental Health Hazard Assessment (OEHHA) (2011). Appendix B: Chemical-specific summaries of the information used to derive unit risk and cancer potency values.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5155632			
EXTRACTION				
Parameter	Data			
Boiling Point	-4.4 C			
CASRN and Test Material	106-99-0; 1,3-BUTADIENE			
Confidentiality, Type, and Guideline	none; not specified; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Standard Deviation Results	NR			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Citing HSDB, 1998.

Study Citation:	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5155603			
EXTRACTION				
Parameter	Data			
Boiling Point	-4.4 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: No source cited; extracted gray lit

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

EXTRACTION	
Parameter	Data
Boiling Point	-4.41 - C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	none; not specified; not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Standard Deviation Results	not reported
Results Details	@ 760 mm Hg

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

Overall Quality Determination

High

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

Study Citation:	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.
OECD Harmonized Template:	Boiling Point
HERO ID:	5160048

EXTRACTION	
Parameter	Data
Boiling Point	-4.44 - C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from Mackay, D., W.Y. Shiu and K.C. Ma. 1993. Illustrated handbook of physical-chemical properties and environmental fate of organic compounds. Vol. III. Lewis Publishers Inc., Chelsea, Michigan.

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5155560			
EXTRACTION				
Parameter	Data			
Boiling Point	-4.9 - C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used
Domain 3: Other	Metric 5:	Databases	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: cited from BASF safety data sheet

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for 1,3-butadiene. CAS Registry Number: 106-99-0..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926412

EXTRACTION	
Parameter	Data
Boiling Point	-4.41 - -4.6 C
CASRN and Test Material	106-99-0; 1,3-Butadiene
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	@ 760 torr; 15 values were reported in Reaxys; 3 of these values were reported in the range of -4.41 to -4.6 C at 760 torr; 12 values were outside this range or measured at unreported or non-standard pressures.

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

Overall Quality Determination **High**

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

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.
OECD Harmonized Template:	Boiling Point
HERO ID:	9493526

EXTRACTION	
Parameter	Data
Boiling Point	Not Reported
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	Not Reported; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	Not Reported
Results Details	critical temperature: 425 K

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

Overall Quality Determination

High

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.
OECD Harmonized Template:	Boiling Point
HERO ID:	9493542

EXTRACTION	
Parameter	Data
Boiling Point	Not Reported
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	Not Reported
Results Details	critical temperature=152 C

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

Overall Quality Determination

High

* Related References: cited from F. O. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953.

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	9493542			
EXTRACTION				
Parameter	Data			
Boiling Point	14.44 - C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	Not Reported			
Results Details	at 200 kPa			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from F. O. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953.

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	9493542			
EXTRACTION				
Parameter	Data			
Boiling Point	-4.413 - C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	Not Reported			
Results Details	at 101.3 kPa			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from F. O. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953.

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	9493542			
EXTRACTION				
Parameter	Data			
Boiling Point	21 - C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	Not Reported			
Results Details	at 245 kPa			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from R. W. Gallant, Hydrocarbon Process. Pet. Refiner 44(10), 151 (1965).

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10171483			
EXTRACTION				
Parameter	Data			
Boiling Point	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Critical Temperature 161.8 C			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 267 (HERO ID: 5926379)

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	192177			
EXTRACTION				
Parameter	Data			
Boiling Point	24 - F			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; None			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Standard Deviation Results	NR			
Results Details	at 1 atmosphere			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	268.7 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	0.4 K			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Hooper, J.H.D., The analysis of hydrocarbon gases by low temperature distillation, Analyst (London), 1947, 72, 513-20.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	268.40 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	1.0 K			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Prevost, C., Erythrene and its dibromides, C. R. Hebd. Seances Acad. Sci., 1928, 186, 1209-13.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	268.7 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	268.7 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	0.4 K			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Anonymous, R., , Am. Pet. Inst. Res. Proj. 45, Ohio State Univ., 1958.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	268.7 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Majer, V.; Svoboda, V., Enthalpies of Vaporization of Organic Compounds: A Critical Review and Data Compilation, Blackwell Scientific Publications, Oxford, 1985, 300.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	268.7 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	2 K			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Anonymous, R., , Am. Pet. Inst. Res. Proj. 45, Tech. Rep. 14, No. 1, Ohio State Univ., 1955.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	270.55 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	1.0 K			
Results Details	results were excluded from overall average reported on NIST reference			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Grosse, A.V., Refractive Indices at Low Temperatures, J. Am. Chem. Soc., 1937, 59, 2739-41.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	268.2 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	1.0 K			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Prevost, C., Bull. Soc. Chim. Fr., 1944, 11, 218.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	268.8 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	0.4 K			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Robey, R.F.; Hudson, B.E.; Wiese, H.K., Determination of individual acetylenes in butadiene and in c4 hydrocarbon fractions, Anal. Chem., 1952, 24, 1080-2.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	268.61 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	0.2 K			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Benoliel, R.W., Some Physical Constants of Seven Four-Carbon-Atom Hydrocarbons and Neopentane, M.S. Thesis, Penn. State Univ., Univ. Park, PA, 1941.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Boiling Point	268.7 - K			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	Not Reported; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Standard Deviation Results	0.5 K			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Foehr, E.G.; Fenske, M.R., Magneto-optic Rotation of Hydrocarbons, Ind. Eng. Chem., 1949, 41, 1956.

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926134

EXTRACTION	
Parameter	Data
Boiling Point	-4.5 C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

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

Study Citation:	O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.
OECD Harmonized Template:	Boiling Point
HERO ID:	5926379

EXTRACTION

Parameter	Data
Boiling Point	-4.5 C
CASRN and Test Material	106-99-0; 1,3-Butadiene
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	@ 760 mm Hg

EVALUATION

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

Overall Quality Determination**High**

Study Citation:	O’Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926379			
EXTRACTION				
Parameter	Data			
Boiling Point	160.0 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
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	40 atm			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	O’Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926379			
EXTRACTION				
Parameter	Data			
Boiling Point	15.3 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
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	2 atm			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	O’Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926379			
EXTRACTION				
Parameter	Data			
Boiling Point	47.0 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
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	5 atm			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	O’Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926379			
EXTRACTION				
Parameter	Data			
Boiling Point	76.0 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
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	10 atm			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	O’Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926379			
EXTRACTION				
Parameter	Data			
Boiling Point	114.0 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
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	20 atm			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	O’Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926379			
EXTRACTION				
Parameter	Data			
Boiling Point	139.8 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
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	30 atm			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Boiling Point	-4.5 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Parchem-fine & specialty chemicals

Study Citation:	Rumble, J. R. (2018). Flammability of chemical substances. :16-16 - 16-32.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	6655446			
EXTRACTION				
Parameter	Data			
Boiling Point	-4.6			
CASRN and Test Material	Not Reported; 1,3-Butadiene			
Confidentiality, Type, and Guideline	none; experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Standard Deviation Results	Not reported			
Results Details	Not reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a known data-collection, prepared by experts in the field.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5349186			
EXTRACTION				
Parameter	Data			
Boiling Point	-4.6 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	U.S. EPA, (2002). Health assessment of 1,3-butadiene.			
OECD Harmonized Template:	Boiling Point			
HERO ID:	52153			
EXTRACTION				
Parameter	Data			
Boiling Point	-4.4 C			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	none; not specified; NA			
Solvent, Reactivity, Storage, and Stability	NA; NA; NA; NA			
Radiolabel, Source, State, and Purity	None; NA; NA; NA			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Secondary source referencing: Weast, RC, ed. (1989) CRC handbook of chemistry and physics, 70th ed. Boca Raton, FL: CRC Press, p. C-160.

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..
OECD Harmonized Template:	Boiling Point
HERO ID:	5926160

EXTRACTION	
Parameter	Data
Boiling Point	-4.44 C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: NIOSH

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926160			
EXTRACTION				
Parameter	Data			
Boiling Point	-5.00 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: SynQuest

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..			
OECD Harmonized Template:	Boiling Point			
HERO ID:	5926160			
EXTRACTION				
Parameter	Data			
Boiling Point	-4.40 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a publicly available database that provides references to the original, peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: PhysProp

Study Citation:	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.
OECD Harmonized Template:	Boiling Point
HERO ID:	6389860

EXTRACTION	
Parameter	Data
Boiling Point	Not Reported
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Standard Deviation Results	Not Reported
Results Details	critical temperature: 152 C

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

Overall Quality Determination

High

* Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed, Volume 4. New York, New York: John Wiley and Sons, 1978. (HERO ID 594584) and Hawley, G.G. 1,3-Butadiene. In: The Condensed Chemical Dictionary, 10th ed., New York, New York: Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID 69425)

Study Citation:	Anonymous, (2005). Butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	9493531			
EXTRACTION				
Parameter	Data			
Density	0.6272 - not reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Density Type	specific gravity			
System	Not Reported			
Temperature	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: no references cited

Study Citation:	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.
OECD Harmonized Template:	Density
HERO ID:	5155603

EXTRACTION	
Parameter	Data
Density	0.6211 g/mL
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; Not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	density
System	Not Reported
Temperature	20 C
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: No source cited; extracted gray lit

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.			
OECD Harmonized Template:	Density			
HERO ID:	3981013			
EXTRACTION				
Parameter	Data			
Density	0.6149 -			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	none; not specified; not specified			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Density Type	specific gravity (density of a substance divided by the density of water)			
System	not specified			
Temperature	25°C			
Standard Deviation Results	not reported			
Results Details	not reported			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Density
HERO ID:	5155560

EXTRACTION	
Parameter	Data
Density	0.65 - g/cm3
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	density
System	Not Reported
Temperature	-6 C
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from Merck Index, 11th Edition (1989). (HERO ID: 5185257)and consolidated IUCLID entry

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	5155560			
EXTRACTION				
Parameter	Data			
Density	0.62 - not reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Density Type	density			
System	Not Reported			
Temperature	20 deg C			
Standard Deviation Results	Not Reported			
Results Details	reported as relative density to water at 4 C			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	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: cited from BASF, Huls, Aver safety data sheets

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	5155560			
EXTRACTION				
Parameter	Data			
Density	1.9 - not reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Density Type	Vapor Density			
System	Not Reported			
Temperature	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	at 20 C			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	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: cited from Kirk – Othmer (1991). Encyclopaedia of Chemical Technology, 4th Edition, 1991. (HERO ID: 3006711)

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	5155560			
EXTRACTION				
Parameter	Data			
Density	0.6211 - not reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Density Type	density			
System	Not Reported			
Temperature	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	reported as relative density.			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from consolidated IUCLID entry

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.
OECD Harmonized Template:	Density
HERO ID:	9493526

EXTRACTION	
Parameter	Data
Density	0.646 - g/cm3
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; liquid; Not Reported
Density Type	Density
System	Not Reported
Temperature	0 C
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Density			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Density	0.582 - g/cm3			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; liquid; Not Reported			
Density Type	Density			
System	Not Reported			
Temperature	50 C			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Density			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Density	0.616 - g/cm3			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; liquid; Not Reported			
Density Type	Density			
System	Not Reported			
Temperature	25 C			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Haz-Map (n.d.). Hazardous agents: 1,3-Butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	7681901			
EXTRACTION				
Parameter	Data			
Density	1.87 -			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	none; Not Reported; not specified			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Density Type	vapor density			
System	not reported			
Temperature	not specified			
Standard Deviation Results	not specified			
Results Details	not specified			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are reported for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data are consistent with the subject chemical substance structural features .
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	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. Secondary source citing secondary source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Citation: HSDB - HERO ID 6628926 (not in distiller PChem at time of extraction)

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.
OECD Harmonized Template:	Density
HERO ID:	9493542

EXTRACTION	
Parameter	Data
Density	1.87 - g/L
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	Vapor Density
System	Not Reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: Cited from F. O. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953.

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.			
OECD Harmonized Template:	Density			
HERO ID:	9493542			
EXTRACTION				
Parameter	Data			
Density	0.245 - g/mL			
CASRN and Test Material	106-99-0; Not Reported			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Density Type	Density			
System	Not Reported			
Temperature	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	reported as critical density			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Cited from F. O. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953.

Study Citation:	National Toxicology Program (NTP), (1999). NTP report on carcinogens background document for 1,3-butadiene.
OECD Harmonized Template:	Density
HERO ID:	5160135

EXTRACTION	
Parameter	Data
Density	0.621 - not reported
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	Not Reported
System	Not Reported
Temperature	20 C/ 4 C
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from Lewis, R. J., Sr. 1992. Sax's Dangerous Properties of Industrial Materials. 8th ed., vol. II. Van Nostrand Reinhold, New York, pp. 572-573. (HERO ID 1649)

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.			
OECD Harmonized Template:	Density			
HERO ID:	192177			
EXTRACTION				
Parameter	Data			
Density	0.65 - Not reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; NR			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Density Type	Specific gravity			
System	Not reported			
Temperature	Not Reported			
Standard Deviation Results	NR			
Results Details	liquid at 24 def F			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information
Overall Quality Determination		Medium		

Study Citation:	NIOSH, (2019). NIOSH pocket guide to chemical hazards: 1,3-Butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	7348615			
EXTRACTION				
Parameter	Data			
Density	1.88 not reported			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Density Type	vapor density			
System	Not Reported			
Temperature	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: no references cited

Study Citation:	NIOSH, (1992). Occupational safety and health guideline for butadiene (1,3-butadiene).
OECD Harmonized Template:	Density
HERO ID:	8408503

EXTRACTION	
Parameter	Data
Density	1.9 - not reported
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	vapor density
System	Not Reported
Temperature	at the boiling point of butadiene
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: no references cited

Study Citation:	NIOSH, (1992). Occupational safety and health guideline for butadiene (1,3-butadiene).			
OECD Harmonized Template:	Density			
HERO ID:	8408503			
EXTRACTION				
Parameter	Data			
Density	0.62 - not reported			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Density Type	density			
System	Not Reported			
Temperature	20 C (68 F)			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: no references cited

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.
OECD Harmonized Template:	Density
HERO ID:	10225178

EXTRACTION	
Parameter	Data
Density	4.53 - mol/l
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	density
System	Not Reported
Temperature	Not Reported
Standard Deviation Results	0.10 mol/l
Results Details	reported as critical

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

Overall Quality Determination

High

* Related References: cited from Tsonopoulos, C.; Ambrose, D., Vapor-Liquid Critical Properties of Elements and Compounds. 6. Unsaturated Aliphatic Hydrocarbons, J. Chem.Eng. Data, 1996, 41, 645-656.

Study Citation:	Sun, H. N., Wristers, J. P. (2002). Butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	5349218			
EXTRACTION				
Parameter	Data			
Density	0.5818 - not reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Density Type	Density			
System	Not Reported			
Temperature	50 C			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: The source cites one of six references W. Baker and A. L. Mossman, Matheson Gas Data Book 83, (1980) F. D. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953. R. C. Weast, CRC Handb. Chem. Phys. 70, C161 (1990). C. L. Yaws and P.-Y. Chiang, Chem. Eng. 95(13), 81 (1988). N. Gee, K. Shinsaka, J. P. Dodelet, and G. R. Freeman, J. Chem. Thermodyn. 18, 221 (1986). C. L. Yaws, H.-C. Yang, J. R. Hopper, and K. C. Hansen, Chem. Eng. 97(4), 177 (1990). Vol. 4 BUTADIENE 385 Standard on Explosion Prevention Systems, National Fire Protection Association, NFPA 69, Boston, Mass., 1973.

Study Citation:	Sun, H. N., Wristers, J. P. (2002). Butadiene.
OECD Harmonized Template:	Density
HERO ID:	5349218

EXTRACTION	
Parameter	Data
Density	0.6194 - not reported
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	Density
System	Not Reported
Temperature	25 C
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination	High
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* Related References: The source cites one of six references W. Baker and A. L. Mossman, Matheson Gas Data Book 83, (1980) F. D. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953. R. C. Weast, CRC Handb. Chem. Phys. 70, C161 (1990). C. L. Yaws and P.-Y. Chiang, Chem. Eng. 95(13), 81 (1988). N. Gee, K. Shinsaka, J. P. Dodelet, and G. R. Freeman, J. Chem. Thermodyn. 18, 221 (1986). C. L. Yaws, H.-C. Yang, J. R. Hopper, and K. C. Hansen, Chem. Eng. 97(4), 177 (1990). Vol. 4 BUTADIENE 385 Standard on Explosion Prevention Systems, National Fire Protection Association, NFPA 69, Boston, Mass., 1973.

Study Citation:	Sun, H. N., Wristers, J. P. (2002). Butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	5349218			
EXTRACTION				
Parameter	Data			
Density	0.6452 - not reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Density Type	Density			
System	Not Reported			
Temperature	0 C			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: The source cites one of six references W. Baker and A. L. Mossman, Matheson Gas Data Book 83, (1980) F. D. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953. R. C. Weast, CRC Handb. Chem. Phys. 70, C161 (1990). C. L. Yaws and P.-Y. Chiang, Chem. Eng. 95(13), 81 (1988). N. Gee, K. Shinsaka, J. P. Dodelet, and G. R. Freeman, J. Chem. Thermodyn. 18, 221 (1986). C. L. Yaws, H.-C. Yang, J. R. Hopper, and K. C. Hansen, Chem. Eng. 97(4), 177 (1990). Vol. 4 BUTADIENE 385 Standard on Explosion Prevention Systems, National Fire Protection Association, NFPA 69, Boston, Mass., 1973.

Study Citation:	Sun, H. N., Wristers, J. P. (2002). Butadiene.
OECD Harmonized Template:	Density
HERO ID:	5349218

EXTRACTION	
Parameter	Data
Density	0.6274 - not reported
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	Density
System	Not Reported
Temperature	15 C
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination	High
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* Related References: The source cites one of six references W. Baker and A. L. Mossman, Matheson Gas Data Book 83, (1980) F. D. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953. R. C. Weast, CRC Handb. Chem. Phys. 70, C161 (1990). C. L. Yaws and P.-Y. Chiang, Chem. Eng. 95(13), 81 (1988). N. Gee, K. Shinsaka, J. P. Dodelet, and G. R. Freeman, J. Chem. Thermodyn. 18, 221 (1986). C. L. Yaws, H.-C. Yang, J. R. Hopper, and K. C. Hansen, Chem. Eng. 97(4), 177 (1990). Vol. 4 BUTADIENE 385 Standard on Explosion Prevention Systems, National Fire Protection Association, NFPA 69, Boston, Mass., 1973.

Study Citation:	U.S. EPA, (2002). Health assessment of 1,3-butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	52153			
EXTRACTION				
Parameter	Data			
Density	0.6211 g/mL			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	none; not specified; NA			
Solvent, Reactivity, Storage, and Stability	NA; NA; NA; NA			
Radiolabel, Source, State, and Purity	NA; NA; gas; NA			
Density Type	density			
System	NA			
Temperature	20°C			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1: Representativeness	High	Data are measured or estimated for the subject chemical substance.	
	Metric 2: Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	
Domain 2: Test Reliability	Metric 3: Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.	
	Metric 4: Reliability/Analytical Method	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: Secondary source referencing: Kirshenbaum, I. (1978) Butadiene. In: Kirk-Othmer encyclopedia of chemical technology, 3rd ed., vol. 4. Mark, HF; Othmer, DF; Overberger, CG; et al., eds. New York, NY: John Wiley and Sons, pp. 313-337. and Verschueren, K. (1983) Handbook of environmental data on organic chemicals, 2nd ed. New York, NY: Van Nostrand Reinhold, pp. 295-297.

Study Citation:	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.
OECD Harmonized Template:	Density
HERO ID:	6389860

EXTRACTION	
Parameter	Data
Density	0.245 - g/cm ³
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Density Type	density
System	Not Reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	reported as critical density

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

Overall Quality Determination

High

* Related References: data already entered under HERO ID 7681901 source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed, Volume 4. New York, New York: John Wiley and Sons, 1978. (HERO ID 594584) and Hawley, G.G. 1,3-Butadiene. In: The Condensed Chemical Dictionary, 10th ed., New York, New York: Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID 69425)

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for 1,3-butadiene. CAS Registry Number: 106-99-0..			
OECD Harmonized Template:	Density			
HERO ID:	5926412			
EXTRACTION				
Parameter	Data			
Density	0.6149 - 0.6216 g/cm3			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	20-25°C			
Standard Deviation Results	Not Reported			
Results Details	@20-25°C; 8 values were reported in Reaxys; 3 values were reported in the range of 0.6149 to 0.6216 at 20-25°C; 5 values were outside this range or measured at unreported or non-standard temperatures.			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a secondary database with a references to the peer-reviewed original source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.
OECD Harmonized Template:	Density
HERO ID:	5926134

EXTRACTION	
Parameter	Data
Density	0.6149 g/cm3
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

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

Study Citation:	O’Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.			
OECD Harmonized Template:	Density			
HERO ID:	5926379			
EXTRACTION				
Parameter	Data			
Density	0.650 g/cm3			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	-6°C			
Standard Deviation Results	Not Reported			
Results Details	at -6°C relative to water at 4°C			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Density	0.62 g/cm3			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	20°C			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: SynQuest

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Density			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Density	0.62 g/cm3			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Parchem-fine & specialty chemicals

Study Citation:	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.
OECD Harmonized Template:	Density
HERO ID:	5349186

EXTRACTION	
Parameter	Data
Density	0.6149 g/cm ³
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25°C and > 1 atm
Standard Deviation Results	Not Reported
Results Details	25°C and > 1 atm

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

Overall Quality Determination

High

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.
OECD Harmonized Template:	Density
HERO ID:	5926134

EXTRACTION	
Parameter	Data
Density	1.87
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not specified
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
System	Not reported
Temperature	Not Reported
Standard Deviation Results	Not Reported
Results Details	air = 1

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

Overall Quality Determination

High

* Related References: Grub, J., Loser, E. 2011. Ullmann's Encyclopedia of Industrial Chemistry. 7th Edition. New York, NY: John Wiley & Sons.

Study Citation:	Anonymous (2014). Substance overview for 1,3-butadiene. :1-1.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	9493530			
EXTRACTION				
Parameter	Data			
Vapor Pressure	2477 - hPa			
CASRN and Test Material	106-99-0; Not Reported			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	20 C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Low	The data are from a primary source without expert peer-review or an unknown secondary source without peer-review and references to the original sources.
	Metric 6:	Models	Low	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: no references cited

Study Citation:	CalEPA, (2008). TSD for noncancer RELs - Appendix D.3 Chronic RELs and toxicity summaries using the previous version of the Hot Spots Risk Assessment guidelines (OEHHA 1999).			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	628645			
EXTRACTION				
Parameter	Data			
Vapor Pressure	910 torr			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	none; Not Reported; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	None; NR; gas; NR			
Temperature	20°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Uninformative	The data does not match the data reported in the source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Uninformative		

* Related References: Gray lit referencing HSDB 2000 and CRC 1995; HEROID: 5926134 for HSDB (2003) reports 2052 mm Hg and HEROID: 5349186 for CRC (2018) reports 1912 mm Hg @ 295 K

Study Citation:	California Office of Environmental Health Hazard Assessment (OEHHA) (2011). Appendix B: Chemical-specific summaries of the information used to derive unit risk and cancer potency values.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5155632

EXTRACTION	
Parameter	Data
Vapor Pressure	910 mm Hg
CASRN and Test Material	106-99-0; 1,3-BUTADIENE
Confidentiality, Type, and Guideline	none; not specified; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR
Temperature	20 deg C
System	NR
Standard Deviation Results	NR
Results Details	Not Reported

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

Overall Quality Determination	High
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* Related References: Citing HSDB, 1998.

Study Citation:	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5155603

EXTRACTION	
Parameter	Data
Vapor Pressure	2100 mm Hg
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; Not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: No source cited; extracted gray lit

Study Citation:	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	3981013			
EXTRACTION				
Parameter	Data			
Vapor Pressure	750 - mm Hg			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	none; not specified; not specified			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Temperature	-4.7°C			
System	not reported			
Standard Deviation Results	not reported			
Results Details	not reported			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5160048

EXTRACTION	
Parameter	Data
Vapor Pressure	281 - kPa
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; calculation; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	calculated at 25 C and 101.325 kPa

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

Overall Quality Determination

High

* Related References: cited from Mackay, D., W.Y. Shiu and K.C. Ma. 1993. Illustrated handbook of physical-chemical properties and environmental fate of organic compounds. Vol. III. Lewis Publishers Inc., Chelsea, Michigan

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5155560

EXTRACTION	
Parameter	Data
Vapor Pressure	244.7 - kPa
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	21 C
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	(CRC handbook 1988)

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

Overall Quality Determination

High

* Related References: cited from the CRC Handbook of Chemistry and Physics (1988). Weast RC, Astle MJ, Beyer WH (Eds). CRC Handbook of Chemistry and Physics, 69th Edition. CRC Press Inc. Boca Raton. USA. (HERO ID: 46579)

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	5155560			
EXTRACTION				
Parameter	Data			
Vapor Pressure	856 - mm Hg			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	no; experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	-1.5 C			
System	Mercury Manometer			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Data measured for a structural analogue of the subject chemical substance are consistent with what is expected for the subject chemical substance structural properties, features or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information
Overall Quality Determination		High		

* Related References: cited from Boublik T et al. (1984). The vapour pressures of pure substances. Volume 17. Elsevier Science Publications, Amsterdam, The Netherlands. and Heisig GB (1933). Action of radon on some unsaturated hydrocarbons. III vinylacetylene and butadiene. J Am Chem Soc. 55; 2304.

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	5155560			
EXTRACTION				
Parameter	Data			
Vapor Pressure	240.0 - kPa			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	20 C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Data measured for a structural analogue of the subject chemical substance are consistent with what is expected for the subject chemical substance structural properties, features or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information
Overall Quality Determination		High		

* Related References: CRC Handbook of Chemistry and Physics (1988) ((HERO ID: 46579)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	9493526

EXTRACTION

Parameter	Data
Vapor Pressure	Not Reported
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	critical pressure= 4.32 MPa

EVALUATION

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

Overall Quality Determination**High**

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Vapor Pressure	986.7 - kPa			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	75 C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of Vaporization: 20.86 kJ/mol at 25C			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Vapor Pressure	101.3 - kPa			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	-4.4 C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Vapor Pressure	273.6 - kPa			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	25 C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Vapor Pressure	537.9 - kPa			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	50 C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Vapor Pressure	120.0 - kPa			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	0 C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Vapor Pressure	1733 - kPa			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	100 C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of Vaporization: 22.47 kJ/mol at -4.4 C			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	9493542

EXTRACTION	
Parameter	Data
Vapor Pressure	Not Reported
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	critical pressure= 4.33 MPab

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

Overall Quality Determination

High

* Related References: cited from F. O. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953.

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	9493542			
EXTRACTION				
Parameter	Data			
Vapor Pressure	24.5 - kPaa			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; liquid; Not Reported			
Temperature	21 C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from F. O. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953.

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.				
OECD Harmonized Template:	Vapor Pressure				
HERO ID:	9493542				
EXTRACTION					
Parameter		Data			
Vapor Pressure		Not Reported			
CASRN and Test Material		106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline		no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability		Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Reported; Not Reported			
Temperature		Not Reported			
System		Not Reported			
Standard Deviation Results		Not Reported			
Results Details		Antoine Equation Parameters for calculating vapor pressure in pascal [log10(P) = A - (B / (T + C))];, A=9.74022 (6.85941 for mm Hg), B=935.531, C=239.554			
EVALUATION					
Domain		Metric	Rating	Comments	
Domain 1: Substance		Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
		Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability		Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
		Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other		Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
		Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination			High		

* Related References: cited from . F. O. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953.

Study Citation:	Laird, D. G., Howat, C. S. (1990). Vapor liquid-phase equilibria and molar volumes of the butadiene acetonitrile system from 300-K to 335-K. Fluid Phase Equilibria 60(1-2):173-190.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5736675

EXTRACTION	
Parameter	Data
Vapor Pressure	297600 - 297900 Pa
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	No; NR; NR; NR
Radiolabel, Source, State, and Purity	None; NR; NR; 99.5% by GC Notes: Primary impurities were light components; reduced by degassing prior to use.
Temperature	300.05 K
System	ParoScientific Digiquartz transducer was used instead of the manometer for pressure measurement
Standard Deviation Results	Experimental uncertainty = 0.1kPa
Results Details	Two results reported at 300.05K = 297.9 kPa and 297.6 kPa

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 or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

High

Study Citation:	MAK-Commission, (2012). 1,3-Butadiene [MAK value documentation, 2001]. :51-70.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	9493518

EXTRACTION	
Parameter	Data
Vapor Pressure	2477 - hPa
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	20 C
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: no references cited

Study Citation:	National Toxicology Program (NTP), (1993). NTP technical report on the toxicology and carcinogenesis studies of 1,3-butadiene (CAS no. 106-99-0) in B6C3F1 mice (inhalation studies).
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5160111

EXTRACTION	
Parameter	Data
Vapor Pressure	1900 - mm Hg
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	Not Reported; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	20 C
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: Citing Kirshenbaum, I. (1978). Butadiene. In Kirk-Othmer Encyclopedia of Chemical Technology, Vol. 4, 3rd ed., pp. 313-337. John Wiley and Sons, New York.

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	10171483

EXTRACTION	
Parameter	Data
Vapor Pressure	Not Reported
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Critical pressure 42.6 atm

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

Overall Quality Determination

High

* Related References: cited from O'Neil, M.J. (ed.). The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 267 (HERO ID: 5926379)

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10171483			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Heat of Vaporization: 20.86 kJ/mol at 25 C; 22.47 kJ/mol at -4.41 C			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Cited from Cited from Haynes, W.M. (ed.). CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014-2015, p. 3-76 (HERO ID: 2828348)

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	192177			
EXTRACTION				
Parameter	Data			
Vapor Pressure	2.4 - atm			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR Notes: NR			
Temperature	NR			
System	NR			
Standard Deviation Results	NR			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	NIOSH, (1992). Occupational safety and health guideline for butadiene (1,3-butadiene).
OECD Harmonized Template:	Vapor Pressure
HERO ID:	8408503

EXTRACTION	
Parameter	Data
Vapor Pressure	1840 - mm Hg
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	21 C (69.8 F)
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: no references cited

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	10225178

EXTRACTION	
Parameter	Data
Vapor Pressure	Not Reported
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Enthalpy of vaporization: 22.9 kJ/mol at 395 KCalculated from the vapor pressure data reported by the method of least squares.

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

Overall Quality Determination

High

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

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of Vaporization: 24.7 kJ/mol at 235 K			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Vaughan, William E., THE HOMOGENEOUS THERMAL POLYMERIZATION OF 1,3-BUTADIENE, J. Am. Chem. Soc., 1932, 54, 10, 3863-3876, <https://doi.org/10.1021/ja01349a008>.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of Vaporization: 21.1 kJ/mol			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Reid, Robert C., Handbook on vapor pressure and heats of vaporization of hydrocarbons and related compounds, R. C. Wilhort and B. J. Zwolinski, Texas A Research Foundation. College Station, Texas(1971). 329 pages.\$10.00, AIChE J., 1972, 18, 6, 1278-1278, <https://doi.org/10.1002/aic.690180637> .

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of Vaporization: 22.47 kJ/mol at 268.7 K			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Majer, V.; Svoboda, V., Enthalpies of Vaporization of Organic Compounds: A Critical Review and Data Compilation, Blackwell Scientific Publications, Oxford, 1985, 300.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	0.08141 kJ/mol at 273.15 K, P=119.95 kPa			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Scott, R.B.; Meyers, C.H.; Rands, R.D., Jr.; Brickwedde, F.G.; Bekkedahl, N., Thermodynamic properties of 1,3-butadiene in the solid, liquid, and vapor states, J. Res. NBS, 1945, 35, 39-85.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of vaporization: 23.0 kJ/mol at 285 KCalculated from the vapor pressure data reported by the method of least squares.			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	203 K			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of Vaporization: 25.7 kJ/mol at 203 KCalculated from the vapor pressure data reported by the method of least squares.			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of Vaporization: 23.6 kJ/mol at 261 K.Calculated from the vapor pressure data reported by the method of least squares.			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of Vaporization: 22.4 kJ/mol at 330 KCalculated from the vapor pressure data reported by the method of least squares.			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of vaporization: 21.47 kJ/mol			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Majer, V.; Svoboda, V., Enthalpies of Vaporization of Organic Compounds: A Critical Review and Data Compilation, Blackwell Scientific Publications, Oxford, 1985, 300.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	43.2 - bar			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	1.0 bar			
Results Details	reported as critical vapor pressure.			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Tsonopoulos, C.; Ambrose, D., Vapor-Liquid Critical Properties of Elements and Compounds. 6. Unsaturated Aliphatic Hydrocarbons, J. Chem.Eng. Data, 1996, 41, 645-656.

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Enthalpy of Vaporization: 23.7 kJ/mol at 256 K			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Boublik, T.; Fried, V.; Hala, E., The Vapour Pressures of Pure Substances: Selected Values of the Temperature Dependence of the Vapour Pressures of Some Pure Substances in the Normal and Low Pressure Region, 2nd ed., Elsevier, New York, 1984, 972.

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926134

EXTRACTION	
Parameter	Data
Vapor Pressure	2052 mm Hg
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	25 C
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: Grub, J., Loser, E. 2011. Ullmann's Encyclopedia of Industrial Chemistry. 7th Edition. New York, NY: John Wiley & Sons.

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926255

EXTRACTION	
Parameter	Data
Vapor Pressure	1824 mm Hg
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	2.4 atm

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

Overall Quality Determination

High

* Related References: NIOSH

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Vapor Pressure	1863 mm Hg			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: SynQuest

Study Citation:	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	5349186			
EXTRACTION				
Parameter	Data			
Vapor Pressure	1912 mm Hg			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	295 K			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	255 kPa at 295 K			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer- reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a recognized, peer- reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	3454			
EXTRACTION				
Parameter	Data			
Vapor Pressure	1 - atm			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	No; Not specified; Not reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	-4.5°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Citing Perry, R.H. and D. Green. 1984. Perry's Chemical Handbook. Physical and Chemical Data. 6th ed. McGraw-Hill Book Co., New York. p. 3-62, HERO ID: 6302806.

Study Citation:	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	3454			
EXTRACTION				
Parameter	Data			
Vapor Pressure	2 - atm			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	No; Not specified; Not reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	14.5°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Citing Perry, R.H. and D. Green. 1984. Perry's Chemical Handbook. Physical and Chemical Data. 6th ed. McGraw-Hill Book Co., New York. p. 3-62, HERO ID: 6302806.

Study Citation:	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	3454			
EXTRACTION				
Parameter	Data			
Vapor Pressure	5 - atm			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	No; Not specified; Not reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	47.0°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Citing Perry, R.H. and D. Green. 1984. Perry's Chemical Handbook. Physical and Chemical Data. 6th ed. McGraw-Hill Book Co., New York. p. 3-62, HERO ID: 6302806.

Study Citation:	U.S. EPA, (2002). Health assessment of 1,3-butadiene.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	52153			
EXTRACTION				
Parameter	Data			
Vapor Pressure	1790 mm Hg			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	none; not specified; NA			
Solvent, Reactivity, Storage, and Stability	NA; NA; NA; NA			
Radiolabel, Source, State, and Purity	NA; NA; gas; NA			
Temperature	20°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	239 kPa			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	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: Secondary source referencing: Santodonato, J. (1985) Monograph on human exposure to chemicals in the workplace: 1,3-butadiene (PB86-147261). Washington, DC: U.S. National Technical Information Service.

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..
OECD Harmonized Template:	Vapor Pressure
HERO ID:	5926160

EXTRACTION	
Parameter	Data
Vapor Pressure	2110 mm Hg
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: PhysProp. Daubert, TE and Danner, RP 1985

Study Citation:	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.
OECD Harmonized Template:	Vapor Pressure
HERO ID:	6389860

EXTRACTION	
Parameter	Data
Vapor Pressure	2.0 - atm
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	15.3 C
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed, Volume 4. New York, New York: John Wiley and Sons, 1978. (HERO ID 594584) and Hawley, G.G. 1,3-Butadiene. In: The Condensed Chemical Dictionary, 10th ed., New York, New York: Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID 69425)

Study Citation:	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.		
OECD Harmonized Template:	Vapor Pressure		
HERO ID:	6389860		
EXTRACTION			
Parameter	Data		
Vapor Pressure	Not Reported		
CASRN and Test Material	106-99-0; 1,3-butadiene		
Confidentiality, Type, and Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported		
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported		
Temperature	Not Reported		
System	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	critical pressure: 4.32 MPa (626 psi)		
EVALUATION			
Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1: Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2: Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3: Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4: Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5: Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6: Models	N/A	Rating of this factor is not applicable to this kind of information
Overall Quality Determination		High	

* Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed, Volume 4. New York, New York: John Wiley and Sons, 1978. (HERO ID 594584)and Hawley, G.G. 1,3-Butadiene. In: The Condensed Chemical Dictionary, 10th ed., New York, New York: Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID 69425)

Study Citation:	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.			
OECD Harmonized Template:	Vapor Pressure			
HERO ID:	6389860			
EXTRACTION				
Parameter	Data			
Vapor Pressure	Not Reported			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Heat of vaporization389 J/g (93 cal/g) at 25 C418 J/g (100 cal/g) at bp			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information
Overall Quality Determination		High		

* Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed, Volume 4. New York, New York: John Wiley and Sons, 1978. (HERO ID 594584) and Hawley, G.G. 1,3-Butadiene. In: The Condensed Chemical Dictionary, 10th ed., New York, New York: Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID 69425)

Study Citation:	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.		
OECD Harmonized Template:	Vapor Pressure		
HERO ID:	6389860		
EXTRACTION			
Parameter	Data		
Vapor Pressure	5.0 - atm		
CASRN and Test Material	106-99-0; 1,3-butadiene		
Confidentiality, Type, and Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported		
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported		
Temperature	47.0 C		
System	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	Not Reported		
EVALUATION			
Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1: Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2: Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3: Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4: Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5: Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6: Models	N/A	Rating of this factor is not applicable to this kind of information
Overall Quality Determination		High	

* Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed, Volume 4. New York, New York: John Wiley and Sons, 1978. (HERO ID 594584)and Hawley, G.G. 1,3-Butadiene. In: The Condensed Chemical Dictionary, 10th ed., New York, New York: Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID 69425)

Study Citation:	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.
OECD Harmonized Template:	logKow
HERO ID:	5155603

EXTRACTION	
Parameter	Data
log k_{ow}	1.99
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; Not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

Continued on next page ...

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Study Citation:	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.
OECD Harmonized Template:	logKow
HERO ID:	5155603

		EVALUATION	
Domain	Metric	Rating	Comments

* Related References: No source cited; extracted gray lit

Study Citation:	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.
OECD Harmonized Template:	logKow
HERO ID:	5160048

EXTRACTION	
Parameter	Data
log k_{ow}	1.99
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from Leo, A., P.Y.C. Jow, C. Silipo and C. Hansch.1975. Calculation of hydrophobic constant(log P) from constants. J. Med. Chem.18: 865–868

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	logKow
HERO ID:	5155560

EXTRACTION	
Parameter	Data
log k_{ow}	1.99 -
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	No; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	0.1
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from Sangster J (1989). Partition coefficients of simple organic compounds. J Phys Chem Ref Data. 18; 1111-1229.

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.			
OECD Harmonized Template:	logKow			
HERO ID:	5155560			
EXTRACTION				
Parameter	Data			
log k_{ow}	1.85 -			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; Not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
pH	Not Reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used
Domain 3: Other	Metric 5:	Databases	Low	The data are from a primary source without expert peer-review or an unknown secondary source without peer-review and references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Cites "Company data unpublished (Huls, 1989) "

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.			
OECD Harmonized Template:	logKow			
HERO ID:	5155560			
EXTRACTION				
Parameter	Data			
log k_{ow}	2.22 -			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; calculated; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
pH	Not Reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	obtained results by utilizing the UNIFAC-derived activity coefficients, to which a simple correction regression was applied			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	Low	The algorithm is not publicly available to verify or reproduce the predictions AND/OR statistics on the external validation set are unavailabl
Overall Quality Determination		High		

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.			
OECD Harmonized Template:	logKow			
HERO ID:	5155560			
EXTRACTION				
Parameter	Data			
log k_{ow}	1.902 -			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; calculated; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
System	Not Reported			
pH	Not Reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used
Domain 3: Other	Metric 5:	Databases	Low	The data are from a primary source without expert peer-review or an unknown secondary source without peer-review and references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Cites "Company data unpublished (Huls, 1989) "

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for 1,3-butadiene. CAS Registry Number: 106-99-0..
OECD Harmonized Template:	logKow
HERO ID:	5926412

EXTRACTION	
Parameter	Data
log k_{ow}	1.902
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	1 data point was reported in Reaxys.

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

Overall Quality Determination

High

* Related References: Smith; Perfetti; Garg; Hansch; Food and Chemical Toxicology; vol. 41; nb. 6; (2003); p. 807 - 817

Study Citation:	Mueller, M., Klein, W. (1992). Comparative evaluation of methods predicting water solubility for organic compounds. Chemosphere 25(6):769-782.			
OECD Harmonized Template:	logKow			
HERO ID:	654554			
EXTRACTION				
Parameter	Data			
log k _{ow}	1.9			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Calculation; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	Not reported			
System	Not reported			
pH	Not reported			
Results Details Method	Not reported			
Standard Deviation Results	Not reported			
Results Details	calculated Pow-values -MedChem-Software 1989			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Calculated data consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear.
	Metric 4:	Reliability/Analytical Method	N/A	This matrix is not applicable to this calculated data.
Domain 3: Other	Metric 5:	Databases	N/A	This matrix is not applicable to this calculated data.
	Metric 6:	Models	High	The model had a defined, unambiguous endpoint and the model performance was known.
Overall Quality Determination		High		

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.			
OECD Harmonized Template:	logKow			
HERO ID:	5926134			
EXTRACTION				
Parameter	Data			
log k_{ow}	1.99			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	Not Reported			
System	Not Reported			
pH	Not Reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a publicly available database that provides references to a peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Hansch, C. Leo, A., Hoekman, D. 1995. Exploring QSAR - Hydrophobic, Electronic, and Steric Constants. Washington, DC: American Chemical Society, p. 8.

Study Citation:	Rumble, J. R., Lide, D. R., Bruno, T. J. (2018). Octanol-water partition coefficients. :5-148-5-187.			
OECD Harmonized Template:	logKow			
HERO ID:	5932746			
EXTRACTION				
Parameter	Data			
log <i>k_{ow}</i>	1.99			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	25°C			
System	Not Reported			
pH	Not Reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..			
OECD Harmonized Template:	logKow			
HERO ID:	5926160			
EXTRACTION				
Parameter	Data			
log <i>k_{ow}</i>	1.99			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	Not Reported			
System	Not Reported			
pH	Not Reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a publicly available database that references peer-reviewed original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

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

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..			
OECD Harmonized Template:	logKow			
HERO ID:	5926160			
EXTRACTION				
Parameter	Data			
log <i>k_{ow}</i>	1.99			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	Not Reported			
System	Not Reported			
pH	Not Reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a publicly available database that references peer-reviewed original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: PhysProp. Egon Willighagen

Study Citation:	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.
OECD Harmonized Template:	Water Solubility
HERO ID:	5160048

EXTRACTION	
Parameter	Data
Water Solubility	735 - mg/L
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
System	Not Reported
pH	Not Reported
Results Details Method	Not Reported
Standard Deviation Results	Not Reported
Results Details	experimental at 25 C and 101.325 kPa

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

Overall Quality Determination

High

* Related References: cited from McAuliffe, C. 1966. Solubility in water of paraffin, cycloparaffin, olefin, acetylene, cycloolefin and aromatic hydrocarbons. J. Phys. Chem. 76: 1267–1275.

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Water Solubility
HERO ID:	5155560

EXTRACTION	
Parameter	Data
Water Solubility	0.735 - g/l
CASRN and Test Material	106-99-0; 1,2-Butadiene
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	Not Reported
System	Not Reported
pH	Not Reported
Results Details Method	gas-liquid chromatography
Standard Deviation Results	Not Reported
Results Details	(McAuliffe 1966)

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

Overall Quality Determination

High

* Related References: cited from McAuliffe C (1966). Solubility in water of paraffin, cycloparaffin, oldfin, acetylene, cyclo-olefin and aromatic hydrocarbons. J Phys Chem. 70; 1267-1275. (HERO ID: 5348315)

Study Citation:	Mueller, M., Klein, W. (1992). Comparative evaluation of methods predicting water solubility for organic compounds. Chemosphere 25(6):769-782.			
OECD Harmonized Template:	Water Solubility			
HERO ID:	654554			
EXTRACTION				
Parameter	Data			
Water Solubility	736 mg/L			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Calculation; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	Not reported			
System	Statistical estimation in relation to partition coefficients.			
pH	Not reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Reported as 1.36E-2 mol/L			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Calculated data consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear.
	Metric 4:	Reliability/Analytical Method	N/A	This matrix is not applicable to this calculated data.
Domain 3: Other	Metric 5:	Databases	N/A	This matrix is not applicable to this calculated data.
	Metric 6:	Models	High	The model had a defined, unambiguous endpoint and the model performance was known.
Overall Quality Determination		High		

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.			
OECD Harmonized Template:	Water Solubility			
HERO ID:	5926134			
EXTRACTION				
Parameter	Data			
Water Solubility	735 mg/L			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	20°C			
System	Not Reported			
pH	Not reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a publicly available database that provides references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: McAuliffe, C. 1966. J Phys Chem 70: 1267-75.

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Water Solubility			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Water Solubility	insoluble			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	Not Reported			
System	Not Reported			
pH	Not reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating		Comments
Domain 1: Substance	Metric 1: Representativeness	High	Data are measured or estimated for the subject chemical substance.	
	Metric 2: Appropriateness	Uninformative	The information is not consistent with measured data for the chemical and this is a qualitative result.	
Domain 2: Test Reliability	Metric 3: Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	
	Metric 4: Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.	
Domain 3: Other	Metric 5: Databases	High	Data is from a publicly available database that references a peer-reviewed source.	
	Metric 6: Models	N/A	Rating of this factor is not applicable to this kind of information.	
Overall Quality Determination		Uninformative		

* Related References: NIOSH

Study Citation:	Rumble, J. R. (2018). Aqueous solubility and Henry’s law constants of organic compounds. :5-148 - 5-177.			
OECD Harmonized Template:	Water Solubility			
HERO ID:	5932745			
EXTRACTION				
Parameter	Data			
Water Solubility	733 mg/L			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	25°C			
System	Not Reported			
pH	Not reported			
Results Details Method	Value of solubility for a gas at a partial pressure of 101.325 kPa (1 atm) in equilibrium with the solution. Originally reported as 0.735 g/kg H2O, converted using CRC handbook’s reported water density at 25 C.			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	U.S. EPA, (2002). Health assessment of 1,3-butadiene.			
OECD Harmonized Template:	Water Solubility			
HERO ID:	52153			
EXTRACTION				
Parameter	Data			
Water Solubility	735 mg/L			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	none; not specified; NA			
Solvent, Reactivity, Storage, and Stability	NR; NR; NA; NA			
Radiolabel, Source, State, and Purity	NA; NA; gas; NA			
Temperature	20°C			
System	NA			
pH	NA			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1: Representativeness	High	Data are measured or estimated for the subject chemical substance.	
	Metric 2: Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	
Domain 2: Test Reliability	Metric 3: Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.	
	Metric 4: Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.	
Domain 3: Other	Metric 5: Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.	
	Metric 6: Models	N/A	Rating of this factor is not applicable to this kind of information.	
Overall Quality Determination		Medium		

* Related References: Secondary source referencing: Sax, NI; Lewis, RJ, Sr. (1987) Hawley's condensed chemical dictionary, 11th ed. New York, NY: Van Nostrand Reinhold, p. 177.

Study Citation:	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..			
OECD Harmonized Template:	Water Solubility			
HERO ID:	5926160			
EXTRACTION				
Parameter	Data			
Water Solubility	735 mg/L			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	Not Reported			
System	Not Reported			
pH	Not reported			
Results Details Method	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Reported as 1.36E-2 mol/L			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a publicly available database that provides references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: PhysProp. McAuliffe, C 1966

Study Citation:	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.			
OECD Harmonized Template:	Flash Point			
HERO ID:	5155603			
EXTRACTION				
Parameter	Data			
Flash Point	-76 C			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	No; Not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: No source cited; extracted gray lit

Study Citation:	Coleman, R. S., Alegria, H. A. (2001). 1,3-Butadiene. :1-4.
OECD Harmonized Template:	Flash Point
HERO ID:	9493522

EXTRACTION	
Parameter	Data
Flash Point	< -7 - C
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: no references cited

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.
OECD Harmonized Template:	Flash Point
HERO ID:	5155560

EXTRACTION	
Parameter	Data
Flash Point	-85 - C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; experimental; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	Closed Cup
Standard Deviation Results	Not Reported
Results Details	DIN 51755, Sax and Lewis, 1987

EVALUATION				
Domain	Metric		Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	Medium	Data measured for a structural analogue of the subject chemical substance are consistent with what is expected for the subject chemical substance structural properties, features or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information

Overall Quality Determination

High

* Related References: Sax NI, Lewis RJ (1987). Hawley's Condensed Chemical Dictionary 11th Edition. Van Norstrand Reinhold Co. New York. (HERO ID: 1061025)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.
OECD Harmonized Template:	Flash Point
HERO ID:	9493526

EXTRACTION	
Parameter	Data
Flash Point	-85 - C
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: K€uhn, Birett: Merkblätter Gef € ahrliche Arbeitsstoffe € ,107. Erg.-Lfg. 5/98 – B 059-1.

Study Citation:	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.			
OECD Harmonized Template:	Flash Point			
HERO ID:	9493542			
EXTRACTION				
Parameter	Data			
Flash Point	-76.1 - C			
CASRN and Test Material	109-66-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from R. W. Gallant, Hydrocarbon Process. Pet. Refiner 44(10), 151 (1965).

Study Citation:	NIOSH, (2007). NIOSH pocket guide to chemical hazards.			
OECD Harmonized Template:	Flash Point			
HERO ID:	192177			
EXTRACTION				
Parameter	Data			
Flash Point	-105 - F			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; closed cup			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; Liquid; NR Notes: NR			
System	closed cup			
Standard Deviation Results	NR			
Results Details	NR			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	NIOSH, (1992). Occupational safety and health guideline for butadiene (1,3-butadiene).
OECD Harmonized Template:	Flash Point
HERO ID:	8408503

EXTRACTION	
Parameter	Data
Flash Point	-156 - F
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	also report 105 C

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

Overall Quality Determination

High

* Related References: no references cited

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Flash Point			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Flash Point	-76.111 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
System	Not Reported			
Standard Deviation Results	Not reported			
Results Details	-105°F (-76.1111°C) (Gas, Liquid, None)			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a 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: NIOSH

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Flash Point			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Flash Point	-76 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
System	Not Reported			
Standard Deviation Results	Not reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Oxford University Chemical Safety Data

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Flash Point			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Flash Point	-76 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
System	Not Reported			
Standard Deviation Results	Not reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: SynQuest

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Flash Point			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Flash Point	-75 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
System	Not Reported			
Standard Deviation Results	Not reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	High	Data is from a publicly available database that provides references to the original, peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Sigma-Aldrich

Study Citation:	U.S. EPA, (2002). Health assessment of 1,3-butadiene.			
OECD Harmonized Template:	Flash Point			
HERO ID:	52153			
EXTRACTION				
Parameter	Data			
Flash Point	-76 C			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	none; not specified; NA			
Solvent, Reactivity, Storage, and Stability	NA; NA; NA; NA			
Radiolabel, Source, State, and Purity	NA; NA; gas; NA			
System	NA			
Standard Deviation Results	NA			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	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: Secondary source referencing: Sax, NI; Lewis, RJ, Sr. (1987) Hawley's condensed chemical dictionary, 11th ed. New York, NY: Van Nostrand Reinhold, p. 177.

Study Citation:	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.
OECD Harmonized Template:	Flash Point
HERO ID:	6389860

EXTRACTION	
Parameter	Data
Flash Point	-105 - C
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology, 3rd ed, Volume 4. New York, New York: John Wiley and Sons, 1978. (HERO ID 594584) and Hawley, G.G. 1,3-Butadiene. In: The Condensed Chemical Dictionary, 10th ed., New York, New York: Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID 69425)

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.		
OECD Harmonized Template:	Autoflammability		
HERO ID:	5155560		
EXTRACTION			
Parameter	Data		
Auto-flammability	415 - C		
CASRN and Test Material	106-99-0; 1,3-Butadiene		
Confidentiality, Type, and Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported		
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported		
System	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	reference to DIN 51794		
Results Value	Not Reported		
EVALUATION			
Domain	Metric	Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	High
	Metric 2:	Appropriateness	High
Data are measured or estimated for the subject chemical substance. 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
	Metric 4:	Reliability/Analytical Method	High
There is no indication that the methodology for producing the information was biased towards a particular product or outcome. Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.			
Domain 3: Other	Metric 5:	Databases	High
	Metric 6:	Models	N/A
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.			
Overall Quality Determination		High	

* Related References: cited from BASF safety data sheet

Study Citation:	ECB, (2002). European Union risk assessment report: 1,3-butadiene.			
OECD Harmonized Template:	Autoflammability			
HERO ID:	5155560			
EXTRACTION				
Parameter	Data			
Auto-flammability	415 - 420 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
Results Value	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from Auer (1989). Auer-Technikum, Ausgabe 12, Auer-Gesellschaft mbH, Berlin, 146-151. and Hommel G (1987). Handbuch der gefährlichen Güter, Merkblatt 44, 4 neubearbeitete Auflage, Springer Verlag, Berlin.

Study Citation:	Rumble, J. R. (2018). Flammability of chemical substances. :16-16 - 16-32.			
OECD Harmonized Template:	Autoflammability			
HERO ID:	6655446			
EXTRACTION				
Parameter	Data			
Auto-flammability	420 C			
CASRN and Test Material	Not Reported; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; not specified; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
System	Not reported			
Standard Deviation Results	Not reported			
Results Details	Not reported			
Results Value	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer- reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a known data-collection, prepared by experts in the field.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.			
OECD Harmonized Template:	Autoflammability			
HERO ID:	5349186			
EXTRACTION				
Parameter	Data			
Auto-flammability	420 C			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not specified			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
System	Not reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
Results Value	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer- reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a recognized, peer- reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	Sun, H. N., Wristers, J. P. (2002). Butadiene.
OECD Harmonized Template:	Autoflammability
HERO ID:	5349218

EXTRACTION				
Parameter		Data		
Auto-flammability		417.8 - C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and Guideline		no; not specied; Not Reported		
Solvent, Reactivity, Storage, and Stability		Not Reported; Not Reported; Not Reported; Not Reported		
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Reported; Not Reported		
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
Results Value		Not Reported		

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

Overall Quality Determination	High
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* Related References: The source cites one of six references W. Baker and A. L. Mossman, Matheson Gas Data Book 83, (1980) F. D. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953. R. C. Weast, CRC Handb. Chem. Phys. 70, C161 (1990). C. L. Yaws and P.-Y. Chiang, Chem. Eng. 95(13), 81 (1988). N. Gee, K. Shinsaka, J. P. Dodelet, and G. R. Freeman, J. Chem. Thermodyn. 18, 221 (1986). C. L. Yaws, H.-C. Yang, J. R. Hopper, and K. C. Hansen, Chem. Eng. 97(4), 177 (1990). Vol. 4 BUTADIENE 385 Standard on Explosion Prevention Systems, National Fire Protection Association, NFPA 69, Boston, Mass., 1973.

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.
OECD Harmonized Template:	Viscosity
HERO ID:	9493526

EXTRACTION	
Parameter	Data
Viscosity	0.20 -
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	50 C
Test Conditions	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	Grub, J., Löser, E. (2011). Butadiene. :381-396.			
OECD Harmonized Template:	Viscosity			
HERO ID:	9493526			
EXTRACTION				
Parameter	Data			
Viscosity	0.25 -			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	no; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	25 C			
Test Conditions	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Data measured for a structural analogue of the subject chemical substance are consistent with what is expected for the subject chemical substance structural properties, features or behaviors.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: cited from D. R. Lide: CRC Handbook of Chemistry and Physics, 79th edition, CRC Press, New York, 1998. (HERO ID: 5349247) and C. L. Yaws et al., Chem. Eng. 83 (1976) no. 17, 79 (HERO ID: 5706678)

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.
OECD Harmonized Template:	Viscosity
HERO ID:	5926134

EXTRACTION	
Parameter	Data
Viscosity	0.00754
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	None; Experimental; Not reported
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR
Radiolabel, Source, State, and Purity	NR; NR; NR; NR
Temperature	20°C
Test Conditions	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

* Related References: Braker, W., Mossman, A.. Matheson. 1980. Matheson Gas Data Book. 6th Ed. P. 79.

Study Citation:	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.			
OECD Harmonized Template:	Viscosity			
HERO ID:	5926134			
EXTRACTION				
Parameter	Data			
Viscosity	0.33			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	-40°C			
Test Conditions	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Braker, W., Mossman, A.. Matheson. 1980. Matheson Gas Data Book. 6th Ed. P. 79.

Study Citation:	Elsevier, (2019). Reaxys: physical-chemical property data for 1,3-butadiene. CAS Registry Number: 106-99-0..			
OECD Harmonized Template:	Refractive Index			
HERO ID:	5926412			
EXTRACTION				
Parameter	Data			
Refractive Index	1.4295			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	20°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	9 values were reported in Reaxys; 1 of these values was reported as 1.4295 at 20 C; 8 values were measured at non-standard temperatures.			
Results Details Methods	Not Reported			
Parameter	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a secondary database with a references to the peer-reviewed original source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

* Related References: Data point includes multiple primary sources in REAXYS.

Study Citation:	O’Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.			
OECD Harmonized Template:	Refractive Index			
HERO ID:	5926379			
EXTRACTION				
Parameter	Data			
Refractive Index	1.4223			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	-6°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
Results Details Methods	Not Reported			
Parameter	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	RSC, (2019). ChemSpider: 1,3-Butadiene.			
OECD Harmonized Template:	Refractive Index			
HERO ID:	5926255			
EXTRACTION				
Parameter	Data			
Refractive Index	1.4292			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
Results Details Methods	Not Reported			
Parameter	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		Medium		

* Related References: Parchem-fine & specialty chemicals

Study Citation:	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.			
OECD Harmonized Template:	Refractive Index			
HERO ID:	5349186			
EXTRACTION				
Parameter	Data			
Refractive Index	1.4292			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	-25°C			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
Results Details Methods	Not Reported			
Parameter	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.
OECD Harmonized Template:	Henry's Law
HERO ID:	5160048

EXTRACTION	
Parameter	Data
Henry's Law	7460 - Pa*m3/mol
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, and Guideline	no; calculated; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
pH	Not Reported
System	calculated at 25 C and 101.325 kPa
Standard Deviation Results	Not Reported
Results Details	Not Reported
Results Details Methods	Not Reported

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

Overall Quality Determination

High

* Related References: cited from Mackay, D. and W.Y. Shiu. 1981. A critical review of Henry's law constants for chemicals of environmental interest. J. Phys. Chem. Ref. Data 10: 1175-1199.

Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.
OECD Harmonized Template:	Henry's Law
HERO ID:	10171483

EXTRACTION	
Parameter	Data
Henry's Law	7.36E-2 - atm-cu m/mole
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	Not Reported; Not Reported; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Temperature	25 C
pH	Not Reported
System	Not Reported
Standard Deviation Results	Not Reported
Results Details	Not Reported
Results Details Methods	calculated from the atmospheric vapor pressure (760 mm Hg since it is a gas) and water solubility

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

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Study Citation:	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.
OECD Harmonized Template:	Henry's Law
HERO ID:	10171483

Domain	Metric	EVALUATION Rating	Comments
Overall Quality Determination		High	

* Related References: Cited from US EPA; Estimation Program Interface (EPI) Suite. Ver. 4.11. Nov, 2012. Available from, as of Mar 9, 2015:

Study Citation:	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.			
OECD Harmonized Template:	Henry’s Law			
HERO ID:	10225178			
EXTRACTION				
Parameter	Data			
Henry’s Law	0.014 - 0.016 mol/(kg*bar)			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	No; not specified; Not Reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	Not Reported			
pH	Not Reported			
System	Noted as Henry’s Law Constant (Water Solution)			
Standard Deviation Results	Not Reported			
Results Details	NIST entry notes that it is missing a citation and doesn’t seem well documented.			
Results Details Methods	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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		Low		

* Related References: missing citation

Study Citation:	Rumble, J. R. (2018). Aqueous solubility and Henry’s law constants of organic compounds. :5-148 - 5-177.			
OECD Harmonized Template:	Henry’s Law			
HERO ID:	5932745			
EXTRACTION				
Parameter	Data			
Henry’s Law	7.589E-2 atm m3/mol			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, and Guideline	None; Experimental; Not Reported			
Solvent, Reactivity, Storage, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State, and Purity	NR; NR; NR; NR			
Temperature	25°C			
pH	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Reported as 7.69 kPa m3 mol-1 (converted using 1 kPa = 0.00986923 atm)			
Results Details Methods	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical’s physical/chemical properties.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Determination		High		

Study Citation:	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.			
OECD Harmonized Template:	Henry’s Law			
HERO ID:	3454			
EXTRACTION				
Parameter	Data			
Henry’s Law	0.0617 - atm-m3/mole			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, and Guideline	No; experimental; Not reported			
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported			
Temperature	25°C			
pH	Not Reported			
System	Not Reported			
Standard Deviation Results	Not Reported			
Results Details	Not Reported			
Results Details Methods	Not Reported			
EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliability	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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: Hine. J. and P.K. Mookerjee. 1975. The intrinsic hydrophilic character of organic compounds. Correlations in terms of structural contributions. J. Org. Chem. 40: 292-298. No HERO ID.

Study Citation:	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.
OECD Harmonized Template:	Dielectric Constant
HERO ID:	5349186

EXTRACTION				
Parameter		Data		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
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		
Dielectric Constant		2.050		
Temperature		Not Reported		
System		Not Reported		
Results Value		Not Reported		
Results Details		Not Reported		

EVALUATION				
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured 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/recognize d database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination	High
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Study Citation:	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.
OECD Harmonized Template:	UV and Visible Absorption
HERO ID:	5160048

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	No; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Wave Length Range	230 nm
Light Source, Optical Path Length, and Optical Cell Type	Not Reported; Not Reported; Not Reported
Test Concentration and Reference Substance	Not Reported; Not Reported
Solvent and Solvent pH	Not Reported; Not Reported
Blank Control, Maxima, Lambda Max, and Peak Band Width	Not Reported; Not Reported; Not Reported; Not Reported
Measured Absolute Value and Molar Coefficient	Not Reported; Not Reported
Results Details	insignificant above 230 nm

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

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Study Citation:	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.
OECD Harmonized	UV and Visible Absorption
Template:	
HERO ID:	5160048

		EVALUATION	
Domain	Metric	Rating	Comments
Overall Quality Determination		High	

* Related References: cited from Jaber, H.M., W.R. Mabey, A.T. Liu, T.W. Chou and H.L. Johnson. 1984. Data acquisition for environmental transport and fate screening. SRI International, Menlo Park, California (EPA 600/6-84-009).

Study Citation:	Fahr, A., Nayak, A. K. (1994). Temperature dependent ultraviolet absorption cross sections of 1,3-butadiene and butadiyne. Chemical Physics 189(3):725-731.
OECD Harmonized Template:	UV and Visible Absorption
HERO ID:	5621443

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	no; experimental; Temperature dependent absorption cross sections
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Matheson Gad Products; Not Reported; Not Reported Notes: used it after successive freeze-pump-thaw cycles.
Wave Length Range	160 - 240
Light Source, Optical Path Length, and Optical Cell Type	a one meter, single beam, vacuum monochromatot provided with interchangeable vacuum UV and UV photomultipliers, a deuterium light source, an analog to digital circuitry, computer controlled stepping motor for wavelength control and computerized data acquisition system; Not Reported; Not Reported
Test Concentration and Reference Substance	Not Reported; Not Reported
Solvent and Solvent pH	Not Reported; Not Reported
Blank Control, Maxima, Lambda Max, and Peak Band Width	Not Reported; Not Reported; aprox. 210 based on figure 1; 160-240 nm
Measured Absolute Value and Molar Coefficient Results Details	Not Reported; Not Reported measured at 333 K, 313 K, 295 K, 273 K, 253 K, 233 K, and 218 K

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

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Study Citation:	Fahr, A., Nayak, A. K. (1994). Temperature dependent ultraviolet absorption cross sections of 1,3-butadiene and butadiyne. Chemical Physics 189(3):725-731.
OECD Harmonized Template:	UV and Visible Absorption
HERO ID:	5621443

Domain	Metric	EVALUATION Rating	Comments
Overall Quality Determination		High	

* Related References: no references cited

Study Citation:	Sun, H. N., Wristers, J. P. (2002). Butadiene.
OECD Harmonized Template:	UV and Visible Absorption
HERO ID:	5349218

EXTRACTION	
Parameter	Data
CASRN and Test Material	106-99-0; Not Reported
Confidentiality, Type, and Guideline	no; not specified; Not Reported
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported; Not Reported
Wave Length Range	217
Light Source, Optical Path Length, and Optical Cell Type	Not Reported; Not Reported; Not Reported
Test Concentration and Reference Substance	Not Reported; Not Reported
Solvent and Solvent pH	Not Reported; Not Reported
Blank Control, Maxima, Lambda Max, and Peak Band Width	Not Reported; Not Reported; 217; cm-1
Measured Absolute Value and Molar Coefficient	Not Reported; Not Reported
Results Details	Not Reported

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

Overall Quality Determination

High

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Study Citation:	Sun, H. N., Wristers, J. P. (2002). Butadiene.
OECD Harmonized Template:	UV and Visible Absorption
HERO ID:	5349218

EVALUATION			
Domain	Metric	Rating	Comments
* Related References: The source cites one of six references W. Baker and A. L. Mossman, Matheson Gas Data Book 83, (1980) F. D. Rossini, K. S. Pitzer, R. L. Arnett, R. M. Braun, and G. C. Pimentel, Selected Values of Physical and Thermodynamic Properties of Hydrocarbons and Related Compounds, American Petroleum Institute Research Project 44, Carnegie Press, Pittsburgh, Pa., 1953. R. C. Weast, CRC Handb. Chem. Phys. 70, C161 (1990). C. L. Yaws and P.-Y. Chiang, Chem. Eng. 95(13), 81 (1988). N. Gee, K. Shinsaka, J. P. Dodelet, and G. R. Freeman, J. Chem. Thermodyn. 18, 221 (1986). C. L. Yaws, H.-C. Yang, J. R. Hopper, and K. C. Hansen, Chem. Eng. 97(4), 177 (1990). Vol. 4 BUTADIENE 385 Standard on Explosion Prevention Systems, National Fire Protection Association, NFPA 69, Boston, Mass., 1973.			

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

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

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Term	Definition
RSC	Royal Society of Chemistry
RT	Retention Time
SIDs	Screening Information Dataset
VP	Vapor Pressure
US or USA	United States of America
UV (UV-Vis)	Ultra Violet (UV-Visible)
WHO	World Health Organization