

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.

HERO ID	Reference	Page
Physical Form or State	e	
5155603	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.	9
3981013	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.	10
5160048	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.	11
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	12
7681901	Haz-Map (n.d.). Hazardous agents: 1,3-Butadiene.	13
9493542	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.	14
5160111	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).	15
5160138	National Toxicology Program (NTP), (2016). Report on carcinogens, fifteenth edition: 1,3-butadiene.	16
10171483	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.	17
192177	NIOSH, (2007). NIOSH pocket guide to chemical hazards.	18
8408503	NIOSH, (1992). Occupational safety and health guideline for butadiene (1,3-butadiene).	19
5349218	Sun, H. N., Wristers, J. P. (2002). Butadiene.	20
10293377	U.S. EPA, (1985). Mutagenicity and carcinogenicity assessment of 1,3-butadiene. Review draft.	21
1565	U.S. EPA, (1985). Mutagenicity and carcinogenicity assessment of 1,3-butadiene: Final report.	22
52153	U.S. EPA, (2002). Health assessment of 1,3-butadiene.	23
5926134	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.	24
5926379	O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.	25
5926255	RSC, (2019). ChemSpider: 1,3-Butadiene.	26
5349186	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.	27
5926134	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.	28
5926255	RSC, (2019). ChemSpider: 1,3-Butadiene.	29
Melting Point		
5155632	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.	30
5155603	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.	31
3981013	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.	32
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5160048	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.	33
5926412	Elsevier, (2019). Reaxys: physical-chemical property data for 1,3-butadiene. CAS Registry Number: 106-99-0	34
9493526	Grub, J., Löser, E. (2011). Butadiene. :381-396.	35
9493542	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.	36
5160135	National Toxicology Program (NTP), (1999). NTP report on carcinogens background document for 1,3-butadiene.	37
10171483	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.	38
192177	NIOSH, (2007). NIOSH pocket guide to chemical hazards.	39
10225178	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.	4(
5926134	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.	44
5926379	O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.	45
5926255	RSC, (2019). ChemSpider: 1,3-Butadiene.	47
5349186	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.	49
5926160	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0	50
6389860	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.	50
Boiling Point		
5155632	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.	57
5155603	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.	58
3981013	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.	59
5160048	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.	60
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	61
5926412	Elsevier, (2019). Reaxys: physical-chemical property data for 1,3-butadiene. CAS Registry Number: 106-99-0	62
9493526	Grub, J., Löser, E. (2011). Butadiene. :381-396.	63
9493542	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.	64
10171483	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.	68
192177	NIOSH, (2007). NIOSH pocket guide to chemical hazards.	69
10225178	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.	70
5926134	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.	81
5926379	O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.	82
5926255	RSC, (2019). ChemSpider: 1,3-Butadiene.	89

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6655446	Rumble, J. R. (2018). Flammability of chemical substances. :16-16 - 16-32.	90
5349186	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.	91
52153	U.S. EPA, (2002). Health assessment of 1,3-butadiene.	92
5926160	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0	93
6389860	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.	96
Density		
9493531	Anonymous, (2005). Butadiene.	97
5155603	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.	98
3981013	DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs.	99
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	100
9493526	Grub, J., Löser, E. (2011). Butadiene. :381-396.	104
7681901	Haz-Map (n.d.). Hazardous agents: 1,3-Butadiene.	107
9493542	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.	108
5160135	National Toxicology Program (NTP), (1999). NTP report on carcinogens background document for 1,3-butadiene.	110
192177	NIOSH, (2007). NIOSH pocket guide to chemical hazards.	111
7348615	NIOSH, (2019). NIOSH pocket guide to chemical hazards: 1,3-Butadiene.	112
8408503	NIOSH, (1992). Occupational safety and health guideline for butadiene (1,3-butadiene).	113
10225178	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.	115
5349218	Sun, H. N., Wristers, J. P. (2002). Butadiene.	116
52153	U.S. EPA, (2002). Health assessment of 1,3-butadiene.	120
6389860	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.	121
5926412	Elsevier, (2019). Reaxys: physical-chemical property data for 1,3-butadiene. CAS Registry Number: 106-99-0	122
5926134	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.	123
5926379	O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.	124
5926255	RSC, (2019). ChemSpider: 1,3-Butadiene.	125
5349186	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.	127
5926134	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.	128
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9493530	Anonymous (2014). Substance overview for 1,3-butadiene. :1-1.	129

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5155632	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.	131
5155603	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.	132
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5160048	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.	134
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	135
9493526	Grub, J., Löser, E. (2011). Butadiene. :381-396.	138
9493542	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.	147
5736675	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.	150
9493518	MAK-Commission, (2012). 1,3-Butadiene [MAK value documentation, 2001]. :51-70.	151
5160111	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).	152
10171483	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.	153
192177	NIOSH, (2007). NIOSH pocket guide to chemical hazards.	155
8408503	NIOSH, (1992). Occupational safety and health guideline for butadiene (1,3-butadiene).	156
10225178	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.	157
5926134	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.	169
5926255	RSC, (2019). ChemSpider: 1,3-Butadiene.	170
5349186	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.	172
3454	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.	173
52153	U.S. EPA, (2002). Health assessment of 1,3-butadiene.	176
5926160	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0	177
6389860	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.	178
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5155603	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.	182
5160048	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.	184
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	185

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Elsevier, (2019). Reaxys: physical-chemical property data for 1,3-butadiene. CAS Registry Number: 106-99-0..

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654554	Mueller, M., Klein, W. (1992). Comparative evaluation of methods predicting water solubility for organic compounds. Chemosphere 25(6):769-782.	19
5926134	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.	19
5932746	Rumble, J. R., Lide, D. R., Bruno, T. J. (2018). Octanol-water partition coefficients. :5-148-5-187.	19
5926160	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0	19
Water Solubility		
5160048	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.	19
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	19
654554	Mueller, M., Klein, W. (1992). Comparative evaluation of methods predicting water solubility for organic compounds. Chemosphere 25(6):769-782.	19
5926134	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.	19
5926255	RSC, (2019). ChemSpider: 1,3-Butadiene.	19
5932745	Rumble, J. R. (2018). Aqueous solubility and Henry's law constants of organic compounds. :5-148 - 5-177.	20
52153	U.S. EPA, (2002). Health assessment of 1,3-butadiene.	20
5926160	U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0	20
Flash Point		
5155603	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries.	20
9493522	Coleman, R. S., Alegria, H. A. (2001). 1,3-Butadiene. :1-4.	20
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	20
9493526	Grub, J., Löser, E. (2011). Butadiene. :381-396.	20
9493542	Kerns, M., Henning, S., Rachita, M. (2002). Butadiene polymers. :317-356.	20
192177	NIOSH, (2007). NIOSH pocket guide to chemical hazards.	20
8408503	NIOSH, (1992). Occupational safety and health guideline for butadiene (1,3-butadiene).	20
5926255	RSC, (2019). ChemSpider: 1,3-Butadiene.	21
52153	U.S. EPA, (2002). Health assessment of 1,3-butadiene.	21
6389860	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.	21
Autoflammability		
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	21
6655446	Rumble, J. R. (2018). Flammability of chemical substances. :16-16 - 16-32.	21
5349186	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.	21

1,3-Butadiene

5349218	Sun, H. N., Wristers, J. P. (2002). Butadiene.	22
pKa		
Viscosity		
9493526	Grub, J., Löser, E. (2011). Butadiene. :381-396.	22
5926134	NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.	22
Refractive Index		
5926412	Elsevier, (2019). Reaxys: physical-chemical property data for 1,3-butadiene. CAS Registry Number: 106-99-0	22
5926379	O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.	22
5926255	RSC, (2019). ChemSpider: 1,3-Butadiene.	22
5349186	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.	22
Henry's Law		
5160048	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.	22
10171483	NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene.	23
10225178	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69.	23
5932745	Rumble, J. R. (2018). Aqueous solubility and Henry's law constants of organic compounds. :5-148 - 5-177.	23
3454	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.	23
Nanomaterial Zeta		
Dielectric Constant		
5349186	Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.	23
UV and Visible Absorption		
5160048	EC, (2000). Priority Substances List Assessment Report: 1,3-Butadiene.	23
5621443	Fahr, A., Nayak, A. K. (1994). Temperature dependent ultraviolet absorption cross sections of 1,3-butadiene and butadiyne. Chemical Physics 189(3):725-731.	23
5349218	Sun, H. N., Wristers, J. P. (2002). Butadiene.	24
Other Properties		
Miscellaneous		
List of Abbreviations and Aeronyms fo	on Data Quality Evaluation and Extraction Tables	24

Study Citation:	California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure				
OECD Harmonized	level summaries Physical Form				
Template: HERO ID:	5155603				
			EXTRACTIO	N	
Parameter		Data			
CASRN and Test Material		106-99-0; 1,3-Butadiene			
Confidentiality, Type, and		No; Not specified; Not Reported			
Solvent, Reactivity, Storag		Not Reported; Not Reported; Not Repo	rted; Not Reported		
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Repo	rted; Not Reported		
Results Value	·	Colorless gas	•		
Results Details		Not Reported			
			EVALUATIO	N	
Domain		Metric	Rating	Comments	
Domain 1: Substance					
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.	
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabil	lity				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	
	Metric 4:	Reliability/Analytical Method	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 Quali	ty Determi	nation	High		

^{*} Related References: No source cited; extracted gray lit

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

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

Femplate: HERO ID:				
	5160048			
			EXTRACTIO	N
Parameter		Data		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and G	uideline	No; not specified; Not Reported		
Solvent, Reactivity, Storage,	, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, ar	nd Purity	Not Reported; Not Reported; colorless ga	as at 25 C with a m	nild aromatic odor; Not Reported
Results Value		Not Reported		
Results Details		Not Reported		
			EVALUATION	 N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabilit	ty			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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.

^{*} 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: OECD Harmonized	ECB, (2002). Et Physical Form o	ropean Union risk assessment report: 1, r State	3-butadiene.			
Template: HERO ID:	5155560					
			EXTRACTIO	N		
Parameter		Data				
CASRN and Test Material		106-99-0; 1,3-Butadiene				
Confidentiality, Type, and	Guideline	No; not specified; Not Reported				
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported			
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; colorless ga	as with a mild aron	natic 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.				
			EVALUATIO	V		
Domain		Metric	EVALUATION Rating	N Comments		
		Metric				
Domain Domain 1: Substance	Metric 1:	Metric Representativeness				
	Metric 1: Metric 2:		Rating	Comments		
	Metric 2:	Representativeness	Rating High	Comments Data are measured or estimated for the subject chemical substance.		
Domain 1: Substance	Metric 2:	Representativeness	Rating High	Comments Data are measured or estimated for the subject chemical substance.		
Domain 1: Substance	Metric 2:	Representativeness Appropriateness	Rating High N/A	Comments Data are measured or estimated for the subject chemical substance. Rating of this factor is not applicable to this kind of information.		

* Related References: missing reference

Metric 5:

Metric 6:

Overall Quality Determination

Databases

Models

High

N/A

High

The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and

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

Study Citation: OECD Harmonized	Haz-Map (n.d.) Physical Form). Hazardous agents: 1,3-Butadiene. or State		
Template: HERO ID:	7681901			
			EXTRACTIO)N
Parameter		Data		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guideline	none; not specified; not specified		
Solvent, Reactivity, Storag	ge, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; gas; NR		
Results Value		Colorless gas with a mild aromatic or gas	soline-like odor	
Results Details		liquid below 24°F as a compressed gas		
			EVALUATIO	N .
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 Reliabi	lity			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
		(Method Objectivity)		-
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	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.

Models

Metric 6:

Overall Quality Determination

N/A

High

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

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

Study Citation: OECD Harmonized	Kerns, M., Hen Physical Form	ning, S., Rachita, M. (2002). Butadiene por State	polymers. :317-35	56.
Template:				
HERO ID:	9493542			
			EXTRACTIO	N
Parameter		Data		
CASRN and Test Material		106-99-0: 1.3-Butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a	•			with a mildly aromatic odor; Not Reported
Results Value	·	Not Reported	Č	•
Results Details		Not Reported		
			EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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				
Domain J. Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to 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:		ology Program (NTP), (1993). NTP tech inhalation studies).	nical report on th	ne toxicology and carcinogenesis studies of 1,3-butadiene (CAS no. 106-99-0) in
OECD Harmonized	Physical Form			
Template:	-			
HERO ID:	5160111			
			EXTRACTIO	N
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 Report	rted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; colorless,	noncorrosive gas; N	Not Reported
Results Value		Not Reported		
Results Details		Kirshenbaum, 1978		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	tv Determi	nation	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: OECD Harmonized	National Toxico Physical Form	ology Program (NTP), (2016). Report on or State	carcinogens, fifte	eenth edition: 1,3-butadiene.
Template: HERO ID:	5160138			
			EXTRACTIO	N
Parameter		Data		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storag	e, and Stability	Not Reported; Not Reported; Not Repor	ted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; colorless g	gas with a mild aron	natic or gasoline odor at room temperature; Not Reported
Results Value		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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.

^{*} Related References: no references cited

Femplate: HERO ID: Parameter	10171483			
Parameter				
Parameter			EXTRACTIO	N
		Data		
CASRN and Test Material		106-99-0; Not Reported		
Confidentiality, Type, and Go	uideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage,	and Stability	Not Reported; Not Reported; Not Repor	ted; Not Reported	
Radiolabel, Source, State, an	d Purity	Not Reported; Not Reported; Not Repor	ted; Not Reported 1	Notes: Mild aromatic odor
Results Value		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabilit	y			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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.

^{*} 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: OECD Harmonized NIOSH, (2007). NIOSH pocket guide to chemical hazards.

ECD Harmonized Physical Form or State

Template:

HERO ID: 192177

EXT	D A	α	rT/	U.	N
P/A I I	KA	l . I		.,	N

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 $<24^{\circ}F$; shipped as a liquefied compressed gas

		EVALUATIO	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric	1: Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric	2: Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability			
Metric	3: Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
	(Method Objectivity)		
Metric	4: Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other			
Metric	5: Databases	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 De	termination	High	

Study Citation: OECD Harmonized	NIOSH, (1992) Physical Form of	. Occupational safety and health guideling State	ne for butadiene (1,3-butadiene).
Template: HERO ID:	8408503			
			EXTRACTIO	N
Parameter		Data		
CASRN and Test Material		106-99-0; Not Reported		
Confidentiality, Type, and Guideline		no; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; shipped ur	nder its own vapor p	pressure as a liquified gas; Not Reported
Radiolabel, Source, State, a	and Purity		flammable gas with	a mild aromatic odor. The odor threshold is reported to be 1.1 parts per million parts
Results Value		of air; Not Reported		
Results Details		Not Reported Not Reported		
Results Details		Not Reported		
			EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	ty Determi	nation	High	

^{*} Related References: no references cited

Study Citation: OECD Harmonized Template:	Sun, H. N., Wri Physical Form of	sters, J. P. (2002). Butadiene. or State		
HERO ID:	5349218			
			EXTRACTION	
Parameter		Data		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; noncorrosiv Not Reported	e, colorless, flammable	gas at room temperature and atmospheric pressure with a mildly aromatic odor;
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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	ty Determi	nation	Medium	

^{*} Related References: no references cited

Study Citation: OECD Harmonized	U.S. EPA, (198 Physical Form of	5). Mutagenicity and carcinogenicity assort State	essment of 1,3-bu	ntadiene. Review draft.
Template: HERO ID:	10293377			
			EXTRACTIO	N
Parameter		Data		
CASRN and Test Material		106-99-0; Not Reported		
Confidentiality, Type, and	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report		
Results Value		colorless gas with a slight aromatic odor	at room temperatu	re and pressure
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	he 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 Quali	tv Determi	nation	High	

^{*} Related References: no references cited

Study Citation:
OECD Harmonized

U.S. EPA, (1985). Mutagenicity and carcinogenicity assessment of 1,3-butadiene: Final report. Physical Form or State

Template:

HERO ID: 1565

Parameter	EXTRACTION 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
Radiolabel, Source, State, and Purity	None; NR; NR
Results Value	colorless gas
Results Details	Not Reported

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

Study Citation: OECD Harmonized	U.S. EPA, (200) Physical Form of	2). Health assessment of 1,3-butadiene.		
Template:	riiysicai roiiii (of State		
HERO ID:	52153			
112110 121	02100		EXTED A CITION	
D		Data	EXTRACTION	
Parameter		Data		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guideline	none; not specified; NA		
Solvent, Reactivity, Storage		NA; NA; NA		
Radiolabel, Source, State,		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 Reliabil	litv			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	(Method Objectivity) Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

^{*} Related References: 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: OECD Harmonized	NLM, (2003). I Physical Form	PubChem: Hazardous Substance Data Bar or State	nk: 1,3-Butadien	ne, 106-99-0.
Template: HERO ID:	5926134			
			EXTRACTIO	N
Parameter		Data		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Results Value		gas		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
		(Method Objectivity)		
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available and peer-reviewed database.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	tv Determi	nation	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:
OECD Harmonized

O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.

Physical Form or State

Template:

HERO ID: 5926379

EATRACTION	EXTR	ACTION
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Parameter	EXTRACTION Data
CACDN and Track Material	106 00 0. 1.2 Protediens
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
Radiolabel, Source, State, and Purity	NR; NR; NR
Results Value	colorless gas
Results Details	Not Reported

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

Study Citation: OECD Harmonized	RSC, (2019). C	ChemSpider: 1,3-Butadiene.		
Template:	Thysical Tollin	of State		
HERO ID:	5926255			
			EXTRACTIO	N
Parameter		Data		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	and Purity	NR; NR; NR; NR		
Results Value		gas or pressurized liquid		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (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 Qualit	v Determi	nation	High	

^{*} Related References: Oxford University Chemical Safety Data

Study Citation:
OECD Harmonized

Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8. Physical Form or State

Template:	
HERO ID:	

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

5349186

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

NLM, (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0.

Study Citation:

OECD Harmonized	Physical Form of	or State		
Template: HERO ID:	5926134			
			EXTRACTION	
Parameter		Data		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guideline	None; Experimental; Not report	rted	
Solvent, Reactivity, Storag	ge, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Results Details		colorless, mildly aromatic or g	asoline-like odor	
			EVALUATION	
Domain		Metric	Rating	Comments

			LILUITIO	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliab	oility			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
		(Method Objectivity)		
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.
Domain 3: Other				
	Metric 5:	Databases	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.

* 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. zed Physical Form or State			
OECD Harmonized				
Template:	•			
HERO ID:	5926255			
			EXTRACTIO	N
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		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
D : 0 T (D !: 1:	1.			
Domain 2: Test Reliabi	•			
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.
		(Method Objectivity)		
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.

Medium

N/A

High

original sources.

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

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

* Related References: Oxford University Chemical Safety Data

Metric 5:

Metric 6:

Overall Quality Determination

Databases

Models

Domain 3: Other

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	Melting Point				
Template:					
HERO ID:	5155632				
			EXTRACTIO	N	
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	e, and Stability	NR; NR; NR; NR			
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR Notes: NR			
Results Details Methods		NR			
Standard Deviation Results	3	NR			
Results Details		Not Reported			
			EVALUATIO	N	
Domain		Metric	Rating	Comments	
Domain 1: Substance					
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.	
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.	
Domain 2: Test Reliabil	ity				
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	
Domain 3: Other					
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.	
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.	
Overall Quali	ty Determi	nation	High		

^{*} Related References: Citing HSDB, 1998.

Study Citation:		ifornia Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure				
OECD Harmonized	level summarie Melting Point	S.				
Template:						
HERO ID:	5155603					
			EXTRACTIO	N		
Parameter		Data				
Melting Point		-108.9 °C				
CASRN and Test Material	l	106-99-0; 1,3-Butadiene				
Confidentiality, Type, and		No; Not specified; Not Reported				
Solvent, Reactivity, Storag		Not Reported; Not Reported; Not Report	ted; Not Reported			
Radiolabel, Source, State,	•	Not Reported; Not Reported; Not Report	•			
Results Details Methods		Not Reported	, 1			
Standard Deviation Result	S	Not Reported				
Results Details		Not Reported				
			EVALUATIO	N		
Domain		Metric	Rating	Comments		
Domain 1: Substance						
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.		
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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.		
D	11.			green area of the second secon		
Domain 2: Test Reliabi	•	D 1: 1:1: /II 1: 1	3.6.11			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.		
	Metric 4:	Reliability/Analytical Method	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						
Domain 3. Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.		
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.		
Overall Quali	ty Determi	nation	High			

^{*} Related References: No source cited; extracted gray lit

Study Citation: OECD Harmonized	DOE, (2016). The Melting Point	Fable 1: Chemicals of concern and assoc	iated chemical inf	ormation. PACs.
Template: HERO ID:	3981013			
			EXTRACTIO	N
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	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	and Purity	NR; NR; NR; NR Notes: NR		
Results Details Methods		not reported		
Standard Deviation Results	3	not reported		
Results Details		not reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	tv Determi	nation	High	

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

Study Citation: OECD Harmonized	EC, (2000). Prio	ority Substances List Assessment Report	: 1,3-Butadiene.	
Template:	Wiening Folin			
HERO ID:	5160048			
			EXTRACTIO	N
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		Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,		Not Reported; Not Reported; Not Report	_	
Results Details Methods	·	Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabil	itv			
2. 1000 100000	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Quali	ty Determi	nation	High	

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

Study Citation: OECD Harmonized Template:	Elsevier, (2019 Melting Point). Reaxys: physical-chemical property da	ta for 1,3-butadie	ene. CAS Registry Number: 106-99-0			
HERO ID:	5926412						
			EXTRACTIO	N			
Parameter		Data					
Melting Point		-108.97108.7 °C					
CASRN and Test Material		106-99-0; 1,3-Butadiene					
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported					
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR					
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR					
Results Details Methods		Measured conditions were not reported; data points were outside the range.	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	S	Not Reported					
Results Details		Not Reported					
			EVALUATIO	N			
Domain		Metric	Rating	Comments			
Domain 1: Substance							
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.			
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.			
Domain 2: Test Reliabil	lity						
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.			
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.			
Domain 3: Other							
	Metric 5:	Databases	High	Data is from a 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.			

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

Study Citation:
OECD Harmonized

Grub, J., Löser, E. (2011). Butadiene. :381-396.

Melting Point

Template:

HERO ID: 9493526

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Parameter	Data		
Maria Bara	N. D I		
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		
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 Relial	bility					
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.		
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qual	lity Determ	ination	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: OECD Harmonized Template:	Kerns, M., Hen Melting Point	ning, S., Rachita, M. (2002). Butadiene po	olymers. :317-35	56.
HERO ID:	9493542			
			EXTRACTIO	N
Parameter		Data		
Melting Point		-108.915 - °C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Results Details Methods		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Reported as freezing point in air at 101.3	kPa	
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	ty Determi	nation	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: OECD Harmonized	National Toxico Melting Point	ology Program (NTP), (1999). NTP repor	t on carcinogens	background document for 1,3-butadiene.
Template: HERO ID:	5160135			
			EXTRACTIO	N
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		Not Reported; Not Reported; Not Report	ted: Not Reported	
Radiolabel, Source, State, a		Not Reported; Not Reported; Not Report	_	
Results Details Methods	·	Not Reported	, 1	
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	tv Determi	nation	High	

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

Study Citation: OECD Harmonized	NCBI, (2020). I Melting Point	PubChem Compound Summary for CID 7	7845 1,3 Butadie	ne.
Template:	Westing Four			
HERO ID:	10171483			
			EXTRACTIO	N
Parameter		Data		
Melting Point		Not Reported		
CASRN and Test Material		106-99-0; 1,3-butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	, and Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State, a	nd Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Results Details Methods		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Enthalpy of fusion: 7.98 kJ/mol		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabili	ty			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Qualit	D 4		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:
OECD Harmonized

NIOSH, (2007). NIOSH pocket guide to chemical hazards.

Melting Point

Template:

ACTION

	EATRACTION
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
Radiolabel, Source, State, and Purity	NR; NR; NR Notes: NR
Results Details Methods	NR
Standard Deviation Results	NR
Results Details	Reported as freezing point

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliab	ility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	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.
011 015	24 D - 4	• 4 •	TT! _1_	
Overall Quali	ity Determ	ınauon	High	

Study Citation: OECD Harmonized Template:	NIST, (2022). N Melting Point	NIST Chemistry WebBook. 1,3-Butadiene	(106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
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	e, and Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Results Details Methods		Not Reported		
Standard Deviation Results		0.2 K		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Quali	ty Dotormi	nation	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: OECD Harmonized	NIST, (2022). Melting Point	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
Template: HERO ID:	10225178			
HERO ID.	10223176			
Danamatan		Data	EXTRACTIO	N
Parameter		Data		
Melting Point		164.210 - K		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	No; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Results Details Methods		Not Reported		
Standard Deviation Results	3	0.04 K		
Results Details		Also report 164.210 K with standard dev	iation of 0.03 K in	same chart under melting point.
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance			<u> </u>	
	Metric 1:	Representativeness	High	Data 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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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.

^{*} 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.

Overall Quality Determination

Study Citation: OECD Harmonized	NIST, (2022). N Melting Point	NIST Chemistry WebBook. 1,3-Butadiene	(106-99-0). Sta	ndard Reference Database No. 69.
Template:	10005170			
HERO ID:	10225178			
_		_	EXTRACTIO	N
Parameter		Data		
Melting Point		164.3 - K		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	No; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Results Details Methods		Not Reported		
Standard Deviation Results		0.4 K		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	Dotomi		High	

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

Study Citation: OECD Harmonized	NIST, (2022). N Melting Point	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
Template:	mening I omi			
HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Melting Point		164.220 - K		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	No; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Results Details Methods		Not Reported		
Standard Deviation Results	S	0.04 K		
Results Details		Also report 164.230 K with standard dev	iation of 0.02 K in	same chart under melting point.
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit			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: OECD Harmonized	Melting Point	PubChem: Hazardous Substance Data Ba	am. 1,5 Buudien	2, 100 // 0.
Template: HERO ID:	5926134			
			EXTRACTIO	N
Parameter		Data		
Melting Point		-108.966 °C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR		
Radiolabel, Source, State, a	and Purity	NR; NR; NR; NR		
Results Details Methods		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	v Determi	nation	High	

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

HERO ID:	5926379			
	3920319			
		.	EXTRACTIO	N
Parameter		Data		
Melting Point		-108.966 °C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage, and Stability		NR; NR; NR		
Radiolabel, Source, State, a	nd Purity	NR; NR; NR; NR		
Results Details Methods		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabili	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				

N/A

High

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

Metric 6:

Overall Quality Determination

Models

Study Citation: OECD Harmonized O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.

Melting Point

Template:

HERO ID: 5926379

EXTRACTION

		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			

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
Me	etric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Me	etric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability				
Me	etric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
Me	etric 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				
Me	etric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
Me	etric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination High

Study Citation: OECD Harmonized	RSC, (2019). C Melting Point	ChemSpider: 1,3-Butadiene.		
Template: 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	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	and Purity	NR; NR; NR; NR		
Results Details Methods		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	tv Determi	nation	Medium	

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

Study Citation: OECD Harmonized	RSC, (2019). C Melting Point	ChemSpider: 1,3-Butadiene.		
Template:	wiching I omic			
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, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Results Details Methods		Not Reported		
Standard Deviation Results	3	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	tv Determi	nation	Medium	

 $^{^\}star$ Related References: Parchem-fine & specialty chemicals

Study Citation: OECD Harmonized	Rumble, J. R., (Melting Point	Ed.) (2018). 1,3-Butadiene. :3-8.		
Template: HERO ID:	5349186			
			EXTRACTIO	N
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, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Results Details Methods		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a 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

Study Citation: OECD Harmonized Template:	U.S. EPA, (201 Melting Point	9). Chemistry Dashboard Information for	1,3-Butadiene.	106-99-0
HERO ID:	5926160			
			EXTRACTIO	N
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, Storag		NR; NR; NR		
Radiolabel, Source, State,		NR; NR; NR; NR		
Results Details Methods	•	Not Reported		
Standard Deviation Result	s	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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				
Zomani J. Onioi	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.

^{*} Related References: PhysProp

Study Citation: OECD Harmonized		9). Chemistry Dashboard Information for	1,3-Butadiene.	106-99-0
OECD Harmonized Template:	Melting Point			
HERO ID:	5926160			
ILIKO ID.	3,20100		EVED ACTIO	NT
Parameter		Data	EXTRACTIO	N
1 ai ainetei		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	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a		NR; NR; NR; NR		
Results Details Methods		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N.
Domain		Metric	Rating	Comments
Domain 1: Substance			<u> </u>	
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	itv			
2. Tool Render	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that references a peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	ty Dotomi	nation	High	

^{*} Related References: NIOSH

Study Citation: OECD Harmonized	U.S. EPA, (201 Melting Point	9). Chemistry Dashboard Information for	1,3-Butadiene. 106-9	99-0
Template:	Wiching I om			
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, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Results Details Methods		Not Reported		
Standard Deviation Results	8	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

Medium

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

Study Citation: OECD Harmonized		9). Chemistry Dashboard Information fo	r 1,3-Butadiene. 106-9	9-0
	Melting Point			
Template: HERO ID:	5026160			
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	e, and Stability	NR; NR; NR		
Radiolabel, Source, State, a		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			<u> </u>	
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	ty Determi	nation	Medium	

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

Study Citation: OECD Harmonized		19). Chemistry Dashboard Information fo	r 1,3-Butadiene. 106-9	99-0
Template:	Melting Point			
HERO ID:	5926160			
TIERO ID.	3720100			
D 4		D 4	EXTRACTION	
Parameter		Data		
Melting Point		-109 °C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR		
Radiolabel, Source, State, a	-	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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	(Method Objectivity) Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was
	MICHIC T.	Remainity// marytical frictiou	Low	used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

^{*} Related References: SynQuest

Overall Quality Determination

Medium

Study Citation: OECD Harmonized	U.S. EPA, (201) Melting Point	9). Chemistry Dashboard Information for	or 1,3-Butadiene. 106-9	99-0
Template:	Wiching I omit			
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, Storag	e, and Stability	NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Results Details Methods		Not Reported		
Standard Deviation Result	S	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	Medium	

^{*} Related References: SynQuest

Study Citation:	U.S. EPA, (1996). Locating and estimating air emissions from sources of 1,3-butadiene.
OECD Harmonized	Melting Point
TD 1 4	

Template:

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	
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported	
Results Details Methods	Not Reported	
Standard Deviation Results	Not Reported	
Results Details	Heat of fusion147.6 J/g (35.28 cal/g)	

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance	;			
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Relial	bility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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.

^{*} Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology,3rd ed, Volume 4. 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; Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID HERO ID: 69425)

	e of Environmental Health Hazard Asse and cancer potency values.	essment (OEHHA) (2011). Appendix B: Chemical-specific summaries of the information used to
	and cancer potency values.	California Office of Environmental Health Hazard Assessment (OEHHA) (2011). Appendix B: Chemical-specific summaries of the information used to	
5155632			
		EXTRACTIO	N .
	Data		
	-4 4 C		
uideline	, ,		
	NR; NR; NR		
nd Purity	NR; NR; NR Notes: NR		
	NR		
	Not Reported		
		EVALUATIO	N
	Metric	Rating	Comments
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
у			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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.
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.
v Determi	nation	High	
	uideline and Stability and Purity Metric 1: Metric 2: iy Metric 3: Metric 4: Metric 5:	Data -4.4 C 106-99-0; 1,3-BUTADIENE none; not specified; Not reported NR; NR; NR; NR NR NR; NR; NR NR Not Reported Metric Metric 1: Representativeness Metric 2: Appropriateness Metric 3: Reliability/Unbiased (Method Objectivity) Metric 4: Reliability/Analytical Method Metric 5: Databases	Data -4.4 C 106-99-0; 1,3-BUTADIENE none; not specified; Not reported and Stability NR; NR; NR; NR NR; NR; NR Notes: NR NR Not Reported Metric Representativeness High Metric 2: Appropriateness High Metric 3: Reliability/Unbiased (Method Objectivity) Metric 4: Reliability/Analytical Method Medium Metric 5: Databases Medium Metric 6: Models N/A

^{*} Related References: Citing HSDB, 1998.

Study Citation:			ssment :: OEHH	A (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure
OECD Harmonized	level summaries Boiling Point	S.		
Template:	Bonnig I ome			
HERO ID:	5155603			
IILKO ID.	3133003			
Parameter		Data	EXTRACTIO	N
rarameter		Data		
Boiling Point		-4.4 C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	No; Not specified; Not Reported		
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Report	ted: Not Reported	
Radiolabel, Source, State, a	•	Not Reported; Not Reported; Not Report		
Standard Deviation Results	•	Not Reported	itea, rvot resportea	
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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.
				below 25 C and a bonning point above 25 C) of behaviors.
Domain 2: Test Reliabili	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased 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				
Domain J. Outer	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	v Determi	nation	High	

^{*} Related References: No source cited; extracted gray lit

Study Citation: OECD Harmonized	DOE, (2016). T Boiling Point	Cable 1: Chemicals of concern and associ	ciated chemical inf	formation. PACs.
Template:				
HERO ID:	3981013			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		-4.41 - C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	none; not specified; not specified		
Solvent, Reactivity, Storage		NR; NR; NR; NR		
Radiolabel, Source, State, a	•	NR; NR; NR; NR Notes: NR		
Standard Deviation Results	3	not reported		
Results Details		@ 760 mm Hg		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	tv Determi	nation	High	

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

Study Citation: OECD Harmonized Template:	EC, (2000). Pri Boiling Point	ority Substances List Assessment Report:	1,3-Butadiene.	
HERO ID:	5160048			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		-4.44 - C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	No; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabili	itv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Qualit	v Determi	nation	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: OECD Harmonized	ECB, (2002). E Boiling Point	European Union risk assessment report: 1,3	3-butadiene.	
Template: HERO ID:	5155560			
			EXTRACTION	
Parameter		Data		
Boiling Point		-4.9 - C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and		no; not specified; Not Reported		
Solvent, Reactivity, Storage	•	Not Reported; Not Reported; Not Reported	•	
Radiolabel, Source, State, a	-	Not Reported; Not Reported; Not Reported	ed; 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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

^{*} Related References: cited from BASF safety data sheet

Study Citation: OECD Harmonized	Elsevier, (2019 Boiling Point). Reaxys: physical-chemical property da	ta for 1,3-butadie	ene. CAS Registry Number: 106-99-0
Template: HERO ID:	5926412			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		-4.414.6 C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Standard Deviation Result	s	Not Reported		
Results Details		@ 760 torr; 15 values were reported in F this range or measured at unreported or r		values were reported in the range of -4.41 to -4.6 C at 760 torr; 12 values were outside ares.
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There 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.

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

Study Citation:	
OECD Harmonized	

Grub, J., Löser, E. (2011). Butadiene. :381-396.

OECD Harmonize

Boiling Point

Template:

TITTE	A COUNTRY	
EXTR	ACTION	

	EATRACTION
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
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported
Standard Deviation Results	Not Reported
Results Details	critical temperature: 425 K

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance	,			
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance 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 Relia	bility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qua	lity Determ	ination	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: OECD Harmonized	Kerns, M., Hen Boiling Point	ning, S., Rachita, M. (2002). Butadiene p	olymers. :317-35	66.
Template: HERO ID:	9493542			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, a	nd Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Standard Deviation Results		Not Reported		
Results Details		critical temperature=152 C		
			EVALUATION	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabil	itv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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.
			N/A	Rating of this factor is not applicable to this kind of information.

^{*} 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.

Overall Quality Determination

Study Citation: OECD Harmonized	Kerns, M., Hen Boiling Point	ning, S., Rachita, M. (2002). Butadiene p	oolymers. :317-35	56.			
Template: HERO ID:	9493542						
			EXTRACTIO	N			
Parameter		Data					
Boiling Point		14.44 - C					
CASRN and Test Material		106-99-0; 1,3-Butadiene					
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported					
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported				
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	Not Reported; Not Reported; Not Reported				
Standard Deviation Results	3	Not Reported					
Results Details		at 200 kPa					
			EVALUATIO	N			
Domain		Metric	Rating	Comments			
Domain 1: Substance							
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.			
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	ity						
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.			
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	ty Determi	nation	High				
Overan Quant	iy Deteriiii	แลนบน	mgn				

^{*} 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: OECD Harmonized	Kerns, M., Hen Boiling Point	ning, S., Rachita, M. (2002). Butadiene p	oolymers. :317-35	56.		
Template: HERO ID:	9493542					
			EXTRACTIO	N		
Parameter		Data				
Boiling Point		-4.413 - C				
CASRN and Test Material		106-99-0; 1,3-Butadiene				
Confidentiality, Type, and		no; not specified; Not Reported				
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Report				
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Reported				
Standard Deviation Results Results Details	S	Not Reported at 101.3 kPa				
Results Details		at 101.5 Ki a				
			EVALUATIO	N		
Domain		Metric	Rating	Comments		
Domain 1: Substance						
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.		
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	lity					
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.		
	Metric 4:	Reliability/Analytical Method	Medium	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.		
Overell Over	ty Dotomos	nation	High			
Overall Quality	ty Determi	แลนงแ	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: OECD Harmonized	Kerns, M., Hen Boiling Point	ning, S., Rachita, M. (2002). Butadiene p	oolymers. :317-3	56.		
Template: HERO ID:	9493542					
			EXTRACTIO	N .		
Parameter		Data				
Boiling Point		21 - C				
CASRN and Test Material		106-99-0; 1,3-Butadiene				
Confidentiality, Type, and		no; not specified; Not Reported				
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Report				
Radiolabel, Source, State,	•	Not Reported; Not Reported; Not Reported				
Standard Deviation Results		Not Reported				
Results Details		at 245 kPa				
			EVALUATIO	N		
Domain		Metric	Rating	Comments		
Domain 1: Substance						
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.		
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	lity					
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.		
	Metric 4:	Reliability/Analytical Method	Medium	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 Over	ty Dotormi	nation	Uigh			
Overall Quality	iy Deterim	แลนงแ	High			

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

Study Citation: OECD Harmonized	NCBI, (2020). I Boiling Point	PubChem Compound Summary for CID 7	7845 1,3 Butadie	ne.
Template:	Bonnig I omt			
HERO ID:	10171483			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Standard Deviation Results		Not Reported		
Results Details		Critical Temperature 161.8 C		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit			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:
OECD Harmonized
Template:

NIOSH, (2007). NIOSH pocket guide to chemical hazards.

Boiling Point

EXTRA	ACTION
LAIN	CHON

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
Radiolabel, Source, State, and Purity	NR; NR; NR Notes: NR
Standard Deviation Results	NR
Results Details	at 1 atmosphere

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance	2			
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Relia	bility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Qua	lity Determ	ination	High	

Study Citation:		NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.			
OECD Harmonized	Boiling Point						
Template:	10005170						
HERO ID:	10225178						
			EXTRACTIO	N			
Parameter		Data					
Boiling Point		268.7 - K					
CASRN and Test Material		106-99-0; 1,3-Butadiene					
Confidentiality, Type, and C	Guideline	Not Reported; Experimental; Not Reported	ed				
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported				
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported				
Standard Deviation Results		0.4 K					
Results Details		Not Reported					
			EVALUATIO	N			
Domain		Metric	Rating	Comments			
Domain 1: Substance							
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.			
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabil	itv						
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome			
	Metric 4:	Reliability/Analytical Method	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 Qualit	ty Determi	nation	High				

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

Template: HERO ID: Parameter Boiling Point CASRN and Test Material		Data 268.40 - K 106-99-0; 1,3-Butadiene Not Reported; Experimental; Not Report	EXTRACTIO	N
Boiling Point		268.40 - K 106-99-0; 1,3-Butadiene	EXTRACTIO	N
Boiling Point		268.40 - K 106-99-0; 1,3-Butadiene		
•		106-99-0; 1,3-Butadiene		
CASRN and Test Material				
		Not Reported: Experimental: Not Papart		
Confidentiality, Type, and G	and Stability	Not Reported, Experimental, Not Report	ed	
Solvent, Reactivity, Storage,	•	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, an	d Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Standard Deviation Results		1.0 K		
Results Details		Not Reported		
			EVALUATIO	 N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabilit	y			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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	v Determi	nation	High	

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

Study Citation: OECD Harmonized	NIST, (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69. Boiling Point 10225178			
Template: HERO ID:				
			EXTRACTIO	N
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		
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance	· · · · · · · · · · · · · · · · · · ·		· · · · · · · · · · · · · · · · · · ·	
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabi	lity			
Domain 2. Test Reliable	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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: OECD Harmonized	NIST, (2022). N Boiling Point	VIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
Template: HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		268.7 - K		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	uideline	Not Reported; Experimental; Not Report	ed	
Solvent, Reactivity, Storage	-	Not Reported; Not Reported; Not Report		
Radiolabel, Source, State, a	nd Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Standard Deviation Results		0.4 K		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabili	ty			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	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 Qualit	-		High	

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

Study Citation: OECD Harmonized	NIST, (2022). N Boiling Point	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	undard Reference Database No. 69.
Template: HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		268.7 - K		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	Not Reported; Experimental; Not Report	ted	
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N .
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	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 Qualit	tv Determi	nation	High	
Overall Qualit	ty Determi	nation	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: OECD Harmonized Femplate:	NIST, (2022). N Boiling Point	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
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 Report		
Solvent, Reactivity, Storage	•	Not Reported; Not Reported; Not Report		
Radiolabel, Source, State, a	nd Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Standard Deviation Results		2 K		
Results Details		Not Reported		
			EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	Uiah	Data and management on actimated for the publicat chamical substance
	Metric 2:	Appropriateness	High 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 (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 Reliabili	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	D 4		High	

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

Study Citation: OECD Harmonized	NIST, (2022). N Boiling Point	NIST Chemistry WebBook. 1,3-Butadiene	(106-99-0). Sta	ndard Reference Database No. 69.
Template: HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		270.55 - K		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	Not Reported; Experimental; Not Reported	ed	
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Standard Deviation Results		1.0 K		
Results Details		results were excluded from overall average	ge reported on NIS	T reference
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit			High	

^{*} Related References: cited fromGrosse, A.V., Refractive Indices at Low Temperatures, J. Am. Chem. Soc., 1937, 59, 2739-41.

Study Citation: OECD Harmonized	NIST, (2022). I Boiling Point	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
Template: HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		268.2 - K		
CASRN and Test Material	1	106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guideline	Not Reported; Experimental; Not Reported	ed	
Solvent, Reactivity, Storag	ge, and Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Standard Deviation Result	S	1.0 K		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabi	lity			
2 omain 2. Test Rendul.	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Quali	tv Determi	nation	High	

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

Study Citation: OECD Harmonized	NIST, (2022). N Boiling Point	VIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
Template: HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		268.8 - K		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	duideline	Not Reported; Experimental; Not Reported	ed	
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Reported		
Radiolabel, Source, State, a	nd Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Standard Deviation Results		0.4 K		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabili	tv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Qualit			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.

Parameter Boiling Point CASRN and Test Material Confidentiality, Type, and Guideline Solvent, Reactivity, Storage, and Stabi Radiolabel, Source, State, and Purity Standard Deviation Results Results Details Domain Domain 1: Substance Metric 2 Domain 2: Test Reliability Metric 2	Data 268.61 - K 106-99-0; 1,3-Butadiene Not Reported; Experimental; Not Report	ted; Not Reported	
Boiling Point CASRN and Test Material Confidentiality, Type, and Guideline Solvent, Reactivity, Storage, and Stabi Radiolabel, Source, State, and Purity Standard Deviation Results Results Details Domain Domain 1: Substance Metric Metric 2 Domain 2: Test Reliability Metric 2	268.61 - K 106-99-0; 1,3-Butadiene Not Reported; Experimental; Not Report ty Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report 0.2 K Not Reported	ted ted; Not Reported ted; Not Reported ted; EVALUATIO	N
Boiling Point CASRN and Test Material Confidentiality, Type, and Guideline Solvent, Reactivity, Storage, and Stabi Radiolabel, Source, State, and Purity Standard Deviation Results Results Details Domain Domain 1: Substance Metric Metric 2 Domain 2: Test Reliability Metric 2	268.61 - K 106-99-0; 1,3-Butadiene Not Reported; Experimental; Not Report ty Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report 0.2 K Not Reported	ted ted; Not Reported ted; Not Reported ted; EVALUATIO	N
CASRN and Test Material Confidentiality, Type, and Guideline Solvent, Reactivity, Storage, and Stabi Radiolabel, Source, State, and Purity Standard Deviation Results Results Details Domain Domain 1: Substance Metric Metric Domain 2: Test Reliability Metric 2	106-99-0; 1,3-Butadiene Not Reported; Experimental; Not Report ty Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report 0.2 K Not Reported	ted; Not Reported ted; Not Reported EVALUATIO	
Confidentiality, Type, and Guideline Solvent, Reactivity, Storage, and Stabi Radiolabel, Source, State, and Purity Standard Deviation Results Results Details Domain Domain 1: Substance Metric Metric Domain 2: Test Reliability Metric 1	Not Reported; Experimental; Not Report Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report 0.2 K Not Reported	ted; Not Reported ted; Not Reported EVALUATIO	
Solvent, Reactivity, Storage, and Stabi Radiolabel, Source, State, and Purity Standard Deviation Results Results Details Domain Domain 1: Substance Metric Metric Domain 2: Test Reliability Metric 1	ty Not Reported; Not Reported; Not Reported; Not Reported; Not Reported; Not Reported; Not Report 0.2 K Not Reported	ted; Not Reported ted; Not Reported EVALUATIO	
Radiolabel, Source, State, and Purity Standard Deviation Results Results Details Domain Domain 1: Substance Metric Metric 2 Domain 2: Test Reliability Metric 2	Not Reported; Not Reported; Not Reported; Not Reported	ted; Not Reported EVALUATIO	
Domain Domain 1: Substance Metric Metric Domain 2: Test Reliability Metric 2	0.2 K Not Reported	EVALUATIO	
Domain Domain 1: Substance Metric Metric Domain 2: Test Reliability Metric	Not Reported		
Domain Domain 1: Substance Metric Metric 2 Domain 2: Test Reliability Metric 2	<u>*</u>		
Domain 1: Substance Metric Metric Domain 2: Test Reliability Metric	Metric		
Domain 1: Substance Metric Metric Domain 2: Test Reliability Metric	Metric	Rating	Comments
Metric Metric 2 Domain 2: Test Reliability Metric 2			
Metric 2 Domain 2: Test Reliability Metric 2			
Domain 2: Test Reliability Metric 2	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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.
Metric 4	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome
	Reliability/Analytical Method	Medium	The analytical method is 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:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
Metric (Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality Det		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: OECD Harmonized Femplate:	NIST, (2022). N Boiling Point	HIST Chemistry WebBook. 1,3-Butadiene	(106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
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		Not Reported; Not Reported; Not Reported		
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Reported	ed; Not Reported	
Standard Deviation Results		0.5 K		
Results Details		Not Reported		
			EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance	M 1	P	TT: 1	
	Metric 1: Metric 2:	Representativeness Appropriateness	High High	Data are measured or estimated for the subject chemical substance. Measured data are consistent with the subject chemical substance structural features
	Metric 2.	Appropriatelless	High	(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 Reliabili	fv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Qualit	D.4		High	

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

Study Citation: OECD Harmonized	NLM, (2003). I Boiling Point	PubChem: Hazardous Substance Data Ba	ank: 1,3-Butadien	e, 106-99-0.
Template: HERO ID:	5926134			
			EXTRACTIO	N
Parameter		Data	EMILITE	•
Dailing Dains		45.0		
Boiling Point CASRN and Test Material		-4.5 C 106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Cuidalina	, ,		
Solvent, Reactivity, Storage		None; Experimental; Not Reported NR; NR; NR; NR		
Radiolabel, Source, State, a		NR; NR; NR; NR		
Standard Deviation Results	•	Not Reported		
Results Details	,	Not Reported		
Results Details		Not reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	litv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There 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 Qualit	tv Determi	nation	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:
OECD Harmonized

O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.

Boiling Point

Template:

HERO ID: 5926379

EXTR	A	CTION	

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
Radiolabel, Source, State, and Purity	NR; NR; NR
Standard Deviation Results	Not Reported
Results Details	@ 760 mm Hg

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

O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.

Template:

Boiling Point

HERO ID:

EX	ΓR.	A(T	TC)N

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	

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliab	ility			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)	3.5.11	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.

O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.

Template:

Boiling Point

HERO ID:

EX	ΓR.	A(T	TC)N

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	
Standard Deviation Results	Not Reported	
Results Details	2 atm	

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

O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.

Template:

Boiling Point

HERO ID:

EX	ΓR.	A(T	TC)N

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	
Radiolabel, Source, State, and Purity	NR; NR; NR	
Standard Deviation Results	Not Reported	
Results Details	5 atm	

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliab	ility			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)	3.5.11	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.

O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.

Template:

Boiling Point

HERO ID:

EX	ΓR.	A(T	TC)N

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	
Standard Deviation Results	Not Reported	
Results Details	10 atm	

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliab	ility			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	3.5	(Method Objectivity)	3.6.12	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.

O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.

OECD Harmonized Template:

Boiling Point

HERO ID:

EXTR		CIT	DT.	\sim	T.T	
H.XIK	A			.,	IN	

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		
Standard Deviation Results	Not Reported		
Results Details	20 atm		

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

O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.

Template:

Boiling Point

HERO ID:

EX	ΓR.	A(T	TC)N

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	
Radiolabel, Source, State, and Purity	NR; NR; NR	
Standard Deviation Results	Not Reported	
Results Details	30 atm	

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliab	ility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a 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: OECD Harmonized	RSC, (2019). C Boiling Point	hemSpider: 1,3-Butadiene.		
Template: HERO ID:	5926255			
112110 121	0,2020		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, Storag		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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	Medium	

 $^{^\}star$ Related References: Parchem-fine & specialty chemicals

Study Citation:	
OECD Harmonized	

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

Boiling Point

Template:

HERO ID: 6655446

$\mathbf{E}\mathbf{X}\mathbf{T}$	RΔ	CT	ION

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
Radiolabel, Source, State, and Purity	NR; NR; NR
Standard Deviation Results	Not reported
Results Details	Not reported

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

Study Citation:	Rumble, J. R., ((Ed.) (2018). 1,3-Butadiene. :3-8.		
OECD Harmonized	Boiling Point			
Template:				
HERO ID:	5349186			
			EXTRACTIO	N
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, Storag		NR; NR; NR		
Radiolabel, Source, State,		NR; NR; NR; NR		
Standard Deviation Result	•	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N .
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabi	litv			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	3.5	D 1: 1:1: /A 1 .: 13.6 .1 1	3.6.11	

Metric 4:

Domain 3: Other

Reliability/Analytical Method

Metric 5: Metric 6: Overall Quality Determ	Databases Models	High N/A High	Data is from a peer-reviewed data collection. Rating of this factor is not applicable to this kind of information.	
Overall Quality Determ		Iligii		

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.

OECD Harmonized	Boiling Point			
Template:	50150			
HERO ID:	52153			
n ,		D .	EXTRACTION	
Parameter		Data		
Boiling Point		-4.4 C		
CASRN and Test Material		106-99-0; 1,3-butadiene		
Confidentiality, Type, and G	uideline	none; not specified; NA		
Solvent, Reactivity, Storage,	, and Stability	NA; NA; NA		
Radiolabel, Source, State, ar	nd 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 Reliabili	tv			
	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.

^{*} 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: OECD Harmonized	U.S. EPA, (201 Boiling Point	9). Chemistry Dashboard Information for	1,3-Butadiene.	106-99-0
Template: HERO ID:	5926160			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		-4.44 C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and		None; Experimental; Not Reported		
Solvent, Reactivity, Storag		NR; NR; NR		
Radiolabel, Source, State,	-	NR; NR; NR; NR		
Standard Deviation Results	•	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance			<u> </u>	
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
2 dinam c. 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.

^{*} Related References: NIOSH

Study Citation: OECD Harmonized	U.S. EPA, (201 Boiling Point	9). Chemistry Dashboard Information for	or 1,3-Butadiene. 106-9	99-0
Template: 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		
Radiolabel, Source, State, and Purity		NR; NR; NR; NR		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	itv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed

Metric 6:

Overall Quality Determination

Models

N/A

Medium

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

^{*} Related References: SynQuest

Study Citation: OECD Harmonized	U.S. EPA, (201 Boiling Point	9). Chemistry Dashboard Information for	1,3-Butadiene.	106-99-0
Template:	Boiling Foilit			
HERO ID:	5926160			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		-4.40 C		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and		None; Experimental; Not Reported		
Solvent, Reactivity, Storag		NR; NR; NR		
Radiolabel, Source, State,		NR; NR; NR; NR		
Standard Deviation Result	s	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Quali	tv Determi	nation	High	

^{*} Related References: PhysProp

Study Citation: OECD Harmonized Template:	U.S. EPA, (199 Boiling Point	6). Locating and estimating air emissions	s from sources of	1,3-butadiene.
HERO ID:	6389860			
			EXTRACTIO	N
Parameter		Data		
Boiling Point		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and		no; not specified; Not Reported		
Solvent, Reactivity, Storage	•	Not Reported; Not Reported; Not Report		
Radiolabel, Source, State, a	•	Not Reported; Not Reported; Not Report	ted; Not Reported	
Standard Deviation Results	S	Not Reported		
Results Details		critical temperature: 152 C		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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

High

Overall Quality Determination

^{*} Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology,3rd ed, Volume 4. 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: Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID HERO ID: 69425)

Study Citation: OECD Harmonized	Anonymous, (2 Density	005). Butadiene.		
Template: 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, Storag	e, and Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Density Type		specific gravity		
System		Not Reported		
Temperature		Not Reported		
Standard Deviation Result	s	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance			-	
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	ty Determi	nation	Medium	

^{*} Related References: no references cited

Study Citation:			essment :: OEHH	A (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure
OECD Harmonized	level summaries Density			
Template:	-			
HERO ID:	5155603			
			EXTRACTIO	N
Parameter		Data		
Density		0.6211 g/mL		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	No; Not specified; Not Reported		
Solvent, Reactivity, Storage	, and Stability	Not Reported; Not Reported; Not Reported	orted; Not Reported	
Radiolabel, Source, State, a	nd Purity	Not Reported; Not Reported; Not Reported	•	
Density Type		density	-	
System		Not Reported		
Temperature	20 C			
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	V
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data 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 Reliabili	itv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Qualit	y Determi	nation	High	

^{*} Related References: No source cited; extracted gray lit

Study Citation: OECD Harmonized	DOE, (2016). T Density	Table 1: Chemicals of concern and associa	ated chemical inf	formation. PACs.		
Template: HERO ID:	3981013					
			EXTRACTIO	N.		
Parameter		Data	EXTRACTIO			
Density		0.6149 -				
CASRN and Test Material		106-99-0; 1,3-Butadiene				
Confidentiality, Type, and	Guideline	none; not specified; not specified				
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR				
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR Notes: NR				
Density Type		specific gravity (density of a substance d	livided by the densi	ity of water)		
System		not specified				
Temperature		25°C				
Standard Deviation Result	s	not reported				
Results Details		not reported				
Domain		Metric	EVALUATIO Rating	Comments		
Domain 1: Substance		Wictie	Kating	Comments		
Domain 1. Substance	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.		
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.		
Domain 2: Test Reliabi	lity					
2 omain 2. Tool Rolland	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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						
Zomani J. Other	Metric 5:	Databases	High	The information or data is 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 Quali	ty Determi	nation	High			

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

Study Citation: OECD Harmonized Template:	ECB, (2002). E Density	European Union risk assessment report: 1,	3-butadiene.	
HERO ID:	5155560			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Report	ted; Not Reported	
Density Type		density		
System		Not Reported		
Temperature		-6 C		
Standard Deviation Result	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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				
2 s.m. 3. S.m.	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	tv Determi	nation	High	

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

Study Citation: OECD Harmonized	ECB, (2002). E Density	European Union risk assessment report: 1,3	-butadiene.	
Template:				
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, Storag		Not Reported; Not Reported; Not Reporte	ed; Not Reported	
Radiolabel, Source, State,	-	Not Reported; Not Reported; Not Reporte	_	
Density Type	•	density		
System		Not Reported		
Temperature		20 deg C		
Standard Deviation Results	S	Not Reported		
Results Details		reported as relative density to water at 4 C		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance			8	
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	litv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Quali	ty Determi	nation	Medium	

^{*} Related References: cited from BASF, Huls, Aver safety data sheets

Study Citation: OECD Harmonized	ECB, (2002). E Density	European Union risk assessment report: 1,3	3-butadiene.	
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		Not Reported; Not Reported; Not Reported	ed: Not Reported	
Radiolabel, Source, State,	-	Not Reported; Not Reported; Not Reported	-	
Density Type	•	Vapor Density	, 1	
System		Not Reported		
Temperature		Not Reported		
Standard Deviation Results	s	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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	ty Determi	nation	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. Density	
· · · · · · · · · · · · · · · · · · ·	
Template:	
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	
Density Type density	
System Not Reported	
Temperature Not Reported	
Standard Deviation Results Not Reported	
Results Details reported as relative density.	
EVALUATION Description	Community
Domain 1: Substance Rating	Comments
	and an artificiated for the continue at the continue and the continue at the c
r · · · · · · · · · · · · · · · · · · ·	ed or estimated for the subject chemical substance.
Metric 2: Appropriateness N/A Rating of this far	ctor is not applicable to this kind of information.
Domain 2: Test Reliability	
•	cation that the methodology for producing the information was biased
· · · · · · · · · · · · · · · · · · ·	ular product or outcome.
Metric 4: Reliability/Analytical Method Medium The analytical m	nethod is non-standard but is expected to be appropriate OR the analyti- known but is likely to be appropriate based on the data's inclusion in a
	ecognized database or other secondary source.
Danielia 2. Odbar	
Domain 3: Other Matria 5: Detabases High The information	and the information of the collection of the col
peer-reviewed by	or data is from a recognized data collection/repository where data are y experts in the field, are broadly available to the public for review and references to the original sources.
	ctor is not applicable to this kind of information.
	**
Overall Quality Determination High	

^{*} Related References: cited from consolidated IUCLID entry

Study Citation: OECD Harmonized Template:	Grub, J., Löser, Density	E. (2011). Butadiene. :381-396.		
HERO ID:	9493526			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ted; 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	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	tv Determi	nation	High	
= : = = =	- J =		8	

^{*} 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: OECD Harmonized Template:	Grub, J., Löser, Density	E. (2011). Butadiene. :381-396.		
HERO ID:	9493526			
			EXTRACTIO	N
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, Storag		Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	-	Not Reported; Not Reported; liquid; Not	•	
Density Type	·	Density	•	
System		Not Reported		
Temperature		50 C		
Standard Deviation Results	s	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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				
2 c 3. Guioi	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	High	

^{*} Related References: 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: OECD Harmonized	Grub, J., Löser, Density	, E. (2011). Butadiene. :381-396.		
Template: HERO ID:	9493526			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ted; 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	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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				
Zomani J. Ouloi	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	tv Determi	ination	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: OECD Harmonized Template:	Haz-Map (n.d.) Density	. Hazardous agents: 1,3-Butadiene.		
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	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	and Purity	NR; NR; NR; NR		
Density Type		vapor density		
System		not reported		
Temperature		not specified		
Standard Deviation Results	3	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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	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 Qualit	ty Determi	nation	Medium	

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

Study Citation: OECD Harmonized Template:	Kerns, M., Hen Density	ning, S., Rachita, M. (2002). Butadiene p	oolymers. :317-35	56.
HERO ID:	9493542			
			EXTRACTIO	N
Parameter		Data		
Density		1.87 - g/L		
CASRN and Test Material	l	106-99-0; Not Reported		
Confidentiality, Type, and	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storag	ge, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Density Type		Vapor Density		
System		Not Reported		
Temperature		Not Reported		
Standard Deviation Result	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N .
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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				
2 3 main 3 1 0 mci	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	High	

^{*} Related References: 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: OECD Harmonized Template:	Kerns, M., Hen Density	ning, S., Rachita, M. (2002). Butadiene p	polymers. :317-35	56.
HERO ID:	9493542			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Density Type		Density		
System		Not Reported		
Temperature		Not Reported		
Standard Deviation Results	s	Not Reported		
Results Details		reported as critical density		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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				
Domain J. Outer	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	High	

^{*} Related References: 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: OECD Harmonized Template:	National Toxico Density	ology Program (NTP), (1999). NTP repor	t on carcinogens	background document for 1,3-butadiene.
HERO ID:	5160135			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Density Type		Not Reported		
System		Not Reported		
Temperature		20 C/ 4 C		
Standard Deviation Result	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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				
Domain 3. Outer	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	tv Determi	nation	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: OECD Harmonized	NIOSH, (2007) Density). NIOSH pocket guide to chemical haza	ırds.	
Template: 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, Storag	ge, 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	S	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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to 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 Quali	tv Determi	nation	Medium	

Study Citation: OECD Harmonized	NIOSH, (2019). Density	. NIOSH pocket guide to chemical hazar	ds: 1,3-Butadiene	e.
Template: HERO ID:	7348615			
			EXTRACTIO	N
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		Not Reported; Not Reported; Not Report	ted: Not Reported	
Radiolabel, Source, State,		Not Reported; Not Reported; Not Report	_	
Density Type	•	vapor density	, 1	
System		Not Reported		
Temperature		Not Reported		
Standard Deviation Results	;	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is 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 Quali	ty Determi	nation	High	

^{*} Related References: no references cited

Study Citation: OECD Harmonized	NIOSH, (1992) Density	. Occupational safety and health guidelin	e for butadiene (1,3-butadiene).
Template: HERO ID:	8408503			
			EXTRACTIO	N
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, Storag		Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,		Not Reported; Not Reported; Not Report	_	
Density Type	•	vapor density		
System		Not Reported		
Temperature		at the boiling point of butadiene		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	ty Determi	nation	High	

^{*} Related References: no references cited

Study Citation: OECD Harmonized	NIOSH, (1992) Density	. Occupational safety and health guidelin	e for butadiene (1,3-butadiene).
Template:	J			
HERO ID:	8408503			
			EXTRACTIO	N
Parameter		Data		
Density		0.62 - not reported		
CASRN and Test Material		106-99-0; 1,3-butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a		Not Reported; Not Reported; Not Report	_	
Density Type	•	density	-	
System		Not Reported		
Temperature		20 C (68 F)		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N .
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	v Determi	nation	High	

^{*} Related References: no references cited

Study Citation: OECD Harmonized Template:	NIST, (2022). N Density	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
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		Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,		Not Reported; Not Reported; Not Report	_	
Density Type	·	density	-	
System		Not Reported		
Temperature		Not Reported		
Standard Deviation Results	S	0.10 mol/l		
Results Details		reported as critical		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is 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				
Zemme. Julei	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	tv Determi	nation	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	Density

Template:

		EXTRACTIO	N
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 Report	ted; Not Reported	
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Density Type	Density		
System	Not Reported		
Temperature	50 C		
Standard Deviation Results	Not Reported		
Results Details	Not Reported		
		EVALUATIO	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	(Method Objectivity)		towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Medium	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.

Overall Quality Determination High

Databases

Models

Metric 5:

Metric 6:

High

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.

^{*} 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: OECD Harmonized	Sun, H. N., Wri Density	isters, J. P. (2002). Butadiene.		
Template: HERO ID:	5349218			
			EXTRACTIO	N
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, Storag		Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Density Type		Density		
System		Not Reported		
Temperature		25 C		
Standard Deviation Result	s	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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

Overall Quality Determination High

Databases

Models

Metric 5:

Metric 6:

Domain 3: Other

High

N/A

peer-reviewed/recognized database or other secondary source.

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

use OR includes references to the original sources.

The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and

^{*} 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: OECD Harmonized	Sun, H. N., Wr Density	isters, J. P. (2002). Butadiene.		
Template: HERO ID:	5349218			
			EXTRACTIO	N
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, Storag	ge, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Density Type		Density		
System		Not Reported		
Temperature		0 C		
Standard Deviation Result	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N .
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)	3.5.11	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				
Domain J. Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and

Overall Quality Determination

Models

Metric 6:

N/A

High

use OR includes references to the original sources.

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

^{*} 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.

ne Stability ity	Data 0.6274 - not reported 106-99-0; 1,3-Butadiene no; not specified; Not Reported Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report Density Not Reported 15 C Not Reported Not Reported Not Reported		
ne Stability	0.6274 - not reported 106-99-0; 1,3-Butadiene no; not specified; Not Reported Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report Density Not Reported 15 C Not Reported	ed; Not Reported ed; Not Reported	
Stability	0.6274 - not reported 106-99-0; 1,3-Butadiene no; not specified; Not Reported Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report Density Not Reported 15 C Not Reported	ed; Not Reported ed; Not Reported	
Stability	0.6274 - not reported 106-99-0; 1,3-Butadiene no; not specified; Not Reported Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report Density Not Reported 15 C Not Reported	ed; Not Reported	N.
Stability	106-99-0; 1,3-Butadiene no; not specified; Not Reported Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report Density Not Reported 15 C Not Reported	ed; Not Reported	N.
Stability	106-99-0; 1,3-Butadiene no; not specified; Not Reported Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report Density Not Reported 15 C Not Reported	ed; Not Reported	N.
Stability	Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report Density Not Reported 15 C Not Reported	ed; Not Reported	N.
Stability	Not Reported; Not Reported; Not Report Not Reported; Not Reported; Not Report Density Not Reported 15 C Not Reported	ed; Not Reported	N.
•	Not Reported; Not Reported; Not Report Density Not Reported 15 C Not Reported	ed; Not Reported	N.
	Density Not Reported 15 C Not Reported	-	N.
	Not Reported 15 C Not Reported	EVALUATIO	N.
	15 C Not Reported	EVALUATIO	N.
	-	EVALUATIO	N.
	-	EVALUATIO	N.
		EVALUATIO	N.
		H.VALUATIO	
	Metric	Rating	Comments
	ivietric	Kating	Comments
ric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
ric 1.	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
110 2.	Appropriateness	IV/A	Kating of this factor is not applicable to this kind of information.
ric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	(Method Objectivity)		towards a particular product or outcome.
ric 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.
ric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
ric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
ri	ic 4:	(Method Objectivity) Reliability/Analytical Method ic 5: Databases	(Method Objectivity) Reliability/Analytical Method Medium ic 5: Databases High ic 6: Models N/A

^{*} 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: OECD Harmonized Template:	U.S. EPA, (200 Density	2). Health assessment of 1,3-butadiene.		
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, Storag	•	NA; NA; NA; NA		
Radiolabel, Source, State,	and Purity	NA; NA; gas; NA		
Density Type		density		
System		NA		
Temperature		20°C		
Standard Deviation Results	3	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.
Domain 2: Test Reliabil	itv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	(Method Objectivity) Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	Medium	

^{*} Related References: 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.andVerschueren, K. (1983) Handbook of environmental data on organic chemicals, 2nd ed. New York, NY:Van Nostrand Reinhold, pp. 295-297.

Study Citation: OECD Harmonized Template:	U.S. EPA, (199 Density	6). Locating and estimating air emissions	from sources of	1,3-butadiene.
HERO ID:	6389860			
			EXTRACTIO	N
Parameter		Data		
Density		0.245 - g/cm3		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a		Not Reported; Not Reported; Not Report	_	
Density Type	Ĭ	density	, 1	
System		Not Reported		
Temperature		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		reported as critical density		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabili	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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.
Overell Oveli	ty Dotomos	nation	IIiak	
Overall Qualit	ly Determi	แลนบน	High	

^{*} Related References: data already entered under HERO ID 7681901source 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 HERO ID: 69425)

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

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

Study Citation: OECD Harmonized	NLM, (2003). I Density	PubChem: Hazardous Substance Data Bar	nk: 1,3-Butadien	ne, 106-99-0.
Template:	•			
HERO ID:	5926134			
			EXTRACTIO	N .
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, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Temperature		25°C		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	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 Quali	tv Determi	nation	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	Density

Template:

HERO ID: 5926379			
		EXTRACTION	N
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		
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	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.

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

Study Citation: OECD Harmonized Template:	RSC, (2019). O Density	ChemSpider: 1,3-Butadiene.		
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, Storag		NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Temperature		20°C		
Standard Deviation Results	3	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	ination	Medium	

^{*} Related References: SynQuest

Study Citation:	RSC, (2019). C	ChemSpider: 1,3-Butadiene.		
OECD Harmonized	Density			
Template:				
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		NR; NR; NR; NR		
Radiolabel, Source, State, a	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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	ty Determi	ination	Medium	

 $^{^\}star$ Related References: Parchem-fine & specialty chemicals

Study Citation: OECD Harmonized Template:	Rumble, J. R., Density	(Ed.) (2018). 1,3-Butadiene. :3-8.		
HERO ID:	5349186			
			EXTRACTIO	N
Parameter		Data		
Density		0.6149 g/cm3		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage, and Stability		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		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	itv			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a recognized, peer-reviewed data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

High

Overall Quality Determination

Study Citation: OECD Harmonized Template:	NLM, (2003). F Density	PubChem: Hazardous Substance Data Ba	nk: 1,3-Butadien	e, 106-99-0.
HERO ID:	5926134			
			EXTRACTIO	N
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	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
System		Not reported		
Temperature		Not Reported		
Standard Deviation Results	3	Not Reported		
Results Details		air = 1		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	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.

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

Study Citation: OECD Harmonized	Anonymous (20 Vapor Pressure	014). Substance overview for 1,3-butadien	e. :1-1.	
Template:	vapor i ressure			
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		Not Reported; Not Reported; Not Reporte	ed: Not Reported	
Radiolabel, Source, State, a	•	Not Reported; Not Reported; Not Reported		
Temperature	Ť	20 C	. 1	
System		Not Reported		
Standard Deviation Results	3	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance	3.6	D	TT' 1	
	Metric 1:	Representativeness	High	Data are measured 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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	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 Qualit	ty Determi	nation	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	Vapor Pressure					
Template:						
HERO ID:	628645					
			EXTRACTION			
Parameter		Data				
Vapor Pressure		910 torr				
CASRN and Test Material		106-99-0; 1,3-butadiene				
	Guidalina	none; Not Reported; Not Reported				
Confidentiality, Type, and Guideline Solvent, Reactivity, Storage, and Stability		NR; NR; NR				
Radiolabel, Source, State,	-	None; NR; gas; NR				
Temperature	and I urity	20°C				
System		Not Reported				
Standard Deviation Results	2	Not Reported				
Results Details	,	Not Reported				
Tresums Detains		Tierreported				
			EVALUATION			
Domain		Metric	Rating	Comments		
Domain 1: Substance						
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.		
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.		
Domain 2: Test Reliabil	litv					
Domain 2. Test Rendon	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased		
	1,100110 01	(Method Objectivity)	1110010111	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						
Domain 5. 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.		
	wichie O.	Models	IVA	Rating of this factor is not applicable to this kind of information.		
Overall Quali	tv Determi	nation	Uninformative			
Over an Quan	ij Dittilli	แนนงน	Ommor matry e			

^{*} 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	Vapor Pressure	and cancer potency values.		
Template:	vapor i ressure			
HERO ID:	5155632			
			EXTRACTIO	AT
Parameter		Data	EXTRACTIO	
1 di dinetti		Duu		
Vapor Pressure		910 mm Hg		
CASRN and Test Material		106-99-0; 1,3-BUTADIENE		
Confidentiality, Type, and C	Guideline	none; not specified; Not reported		
Solvent, Reactivity, Storage		NR; NR; NR		
Radiolabel, Source, State, a	-	NR; NR; NR Notes: NR		
Temperature	,	20 deg C		
System		NR		
Standard Deviation Results		NR		
Results Details		Not Reported		
			EVALUATIO	N .
Domain		Metric	Rating	Comments
Domain 1: Substance			11441115	- Commons
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
D	:4			
Domain 2: Test Reliabil	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was bissed
	Metric 3.	(Method Objectivity)	Mediuiii	There is no indication that 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				
Domain 5: Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	tv Determi	nation	High	

^{*} Related References: Citing HSDB, 1998.

Study Citation:	California Offic	ee of Environmental Health Hazard Asses	sment :: OEHH	A (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure
OECD Harmonized	level summaries Vapor Pressure			
Template:	vapor i ressure			
HERO ID:	5155603			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Temperature		25 C		
System		Not Reported		
Standard Deviation Result	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Quali	ty Dotormi	nation	High	

^{*} Related References: No source cited; extracted gray lit

Study Citation: OECD Harmonized	DOE, (2016). T Vapor Pressure	Table 1: Chemicals of concern and associ	ated chemical inf	Formation. PACs.
Template: HERO ID:	3981013			
			EXTRACTIO	N
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, Storag	e, 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 Result	S	not reported		
Results Details		not reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Quali	ty Determi	nation	High	

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

Study Citation: OECD Harmonized Template:	EC, (2000). Pri Vapor Pressure	ority Substances List Assessment Report:	1,3-Butadiene.	
HERO ID:	5160048			
			EXTRACTIO	N
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, Storag	ge, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Temperature		25 C		
System		Not Reported		
Standard Deviation Result	s	Not Reported		
Results Details		calculated at 25 C and 101.325 kPa		
			EVALUATIO	N .
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabi	litv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Quali	tv Determi	nation	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: OECD Harmonized	ECB, (2002). E Vapor Pressure	European Union risk assessment report: 1,	,3-butadiene.	
Template: HERO ID:	5155560			
			EXTRACTIO	N
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		Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Temperature		21 C		
System		Not Reported		
Standard Deviation Results	3	Not Reported		
Results Details		(CRC handbook 1988)		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information
Overall Quali	ty Determi	nation	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: OECD Harmonized Template:	ECB, (2002). Et Vapor Pressure	uropean Union risk assessment report: 1	,3-butadiene.	
HERO ID:	5155560			
			EXTRACTIO	N .
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	e, and Stability	Not Reported; Not Reported; Not Report	rted; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	rted; Not Reported	
Temperature		-1.5 C		
System		Mercury Manometer		
Standard Deviation Results	;	Not Reported		
Results Details		Not Reported		
			EVALUATION	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	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 Reliabil	itv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Qualit	tv Determi	nation	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: OECD Harmonized	ECB, (2002). European Union risk assessment report: 1,3-butadiene. Vapor Pressure						
Template:	1						
HERO ID:	5155560						
			EXTRACTIO	N			
Parameter		Data					
Vapor Pressure		240.0 - kPa					
CASRN and Test Material		106-99-0; 1,3-butadiene					
Confidentiality, Type, and G	duideline	no; not specified; Not Reported					
Solvent, Reactivity, Storage	, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported				
Radiolabel, Source, State, as	nd Purity	Not Reported; Not Reported; Not Report	ted; Not Reported				
Temperature		20 C					
System		Not Reported					
Standard Deviation Results		Not Reported					
Results Details		Not Reported					
			EVALUATIO	N			
Domain		Metric	Rating	Comments			
Domain 1: Substance							
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.			
	Metric 2:	Appropriateness	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 Reliabili	tv						
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Qualit	v Determir	ation	High				

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

Study Citation:	
OECD Harmonized	

Grub, J., Löser, E. (2011). Butadiene. :381-396.

Vapor Pressure

Template:

HERO ID: 9493526

		EXTRACTIO	N
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 I	Reported: Not Reported	
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not I		
Temperature	Not Reported	reported, 1 tot reported	
System	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	critical pressure= 4.32 MPa		
ъ.	26	EVALUATIO:	
Domain	Metric	Rating	Comments
Domain 1: Substance	D	TT' 1	
Metric 1:	Representativeness	High	Data 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.
Demois 2. Test Delichilita			
Domain 2: Test Reliability	Daliability/Habiasad	Madi	
Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased

Overall Quality Determination		ination	High	
	Metric 6:	Models	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 4:	(Method Objectivity) Reliability/Analytical Method	Medium	towards a particular product or outcome. 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.
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased

^{*} 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: OECD Harmonized		E. (2011). Butadiene. :381-396.		
Template:	Vapor Pressure			
HERO ID:	9493526			
			EXTRACTIO	N .
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		Not Reported; Not Reported; Not Report	ed: Not Reported	
Radiolabel, Source, State,	-	Not Reported; Not Reported; Not Report	_	
Temperature	.	75 C	1	
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
		•		
ъ.			EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance	3.6	D	TT: 1	
	Metric 1:	Representativeness	High	Data 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 Reliabil	litv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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				
2 3 3. Suloi	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Over	tr. Dotows	nation	High	
Overall Quali	ty Determi	เมลนเงเเ	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: OECD Harmonized	Grub, J., Löser, Vapor Pressure	E. (2011). Butadiene. :381-396.				
Template: HERO ID:	9493526					
			EXTRACTIO	N		
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, Storag	e, and Stability	Not Reported; Not Reported; Not Reported				
Radiolabel, Source, State,	and Purity	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				
			EVALUATIO	N		
Domain		Metric	Rating	Comments		
Domain 1: Substance						
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.		
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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.		

				below 25°C and a boiling point above 25°C) or behaviors.
Domain 2: Test Rel	iability			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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.

^{*} 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)

High

Overall Quality Determination

Study Citation: OECD Harmonized	Grub, J., Löser, Vapor Pressure	E. (2011). Butadiene. :381-396.		
Template:	vapor rressare			
HERO ID:	9493526			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		101.3 - kPa		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and		no; not specified; Not Reported		
Solvent, Reactivity, Storag		Not Reported; Not Reported; Not Report	ted: Not Reported	
Radiolabel, Source, State,		Not Reported; Not Reported; Not Report	_	
Temperature	and rainly	-4.4 C	ica, mor responde	
System		Not Reported		
Standard Deviation Result	s	Not Reported		
Results Details		Not Reported		
			EVALUATIO	Ni
Domain		Metric	Rating	Comments
Domain 1: Substance		House	ranng	Comments
2 omain 1. Suostano	Metric 1:	Representativeness	High	Data 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.
				below 23 C and a bonning point above 25 C) of benaviors.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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				
Domain 3. Other	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
0	4 D-4		TT! - 1	
Overall Quali	ty Determi	nauon	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: OECD Harmonized	Grub, J., Löser, Vapor Pressure	E. (2011). Butadiene. :381-396.		
Template:				
HERO ID:	9493526			
			EXTRACTIO	N
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, Storag		Not Reported; Not Reported; Not Report	ted: Not Reported	
Radiolabel, Source, State,	-	Not Reported; Not Reported; Not Report	_	
Temperature	.	25 C	1	
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	ty Dotormi	nation	High	
Overall Quali	ty Determin	เมลนบม	mgn	

^{*} 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: OECD Harmonized	Grub, J., Löser, Vapor Pressure	E. (2011). Butadiene. :381-396.		
Template:	vapoi riessure			
HERO ID:	9493526			
			EXTRACTIO	N
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, Storag		Not Reported; Not Reported; Not Report	ted: Not Reported	
Radiolabel, Source, State,	-	Not Reported; Not Reported; Not Report	_	
Temperature	.	50 C	1	
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance			8	
	Metric 1:	Representativeness	High	Data 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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Ougli	ty Dotormi	nation	High	
Overall Quali	ty Determi	nation	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: OECD Harmonized	Grub, J., Löser, Vapor Pressure	E. (2011). Butadiene. :381-396.		
Template: HERO ID:	9493526			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		120.0 - kPa		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Report	ted: Not Reported	
Radiolabel, Source, State, a		Not Reported; Not Reported; Not Report	•	
Temperature	and I direct	0 C	ica, rioi rioporica	
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	v Determi	nation	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: OECD Harmonized		, E. (2011). Butadiene. :381-396.		
	Vapor Pressure			
Template: HERO ID:	9493526			
			EXTRACTIO	N
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, Storag		Not Reported; Not Reported; Not Report	ted: Not Reported	
Radiolabel, Source, State,	-	Not Reported; Not Reported; Not Report	_	
Temperature		100 C	,	
System		Not Reported		
Standard Deviation Results	s	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N.
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	ty Dotomi	notion	High	
Overall Quali	ty Determin	เมลมบม	mgn	

^{*} 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: OECD Harmonized	Grub, J., Löser, I Vapor Pressure	E. (2011). Butadiene. :381-396.		
Template: HERO ID:	9493526			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	rted; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	rted; 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	
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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

^{*} 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: OECD Harmonized	Kerns, M., Hen Vapor Pressure	ning, S., Rachita, M. (2002). Butadiene p	oolymers. :317-35	56.
Template: HERO ID:	9493542			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C		no; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Temperature		Not Reported		
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		critical pressure= 4.33 MPab		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit		4.	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: OECD Harmonized	Kerns, M., Hen Vapor Pressure	ning, S., Rachita, M. (2002). Butadiene p	oolymers. :317-35	56.
Template: HERO ID:	9493542			
			EXTRACTIO	N
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		Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	-	Not Reported; Not Reported; liquid; Not	•	
Temperature	-	21 C	•	
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	tv Determi	nation	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: OECD Harmonized	Kerns, M., Henr Vapor Pressure	ning, S., Rachita, M. (2002). Butadiene p	oolymers. :317-35	56.
Template:				
HERO ID:	9493542			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a	•	Not Reported; Not Reported; Not Report	•	
Temperature	·	Not Reported	•	
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Antoine Equation Parameters for calculat C=239.554	ting vapor pressure	in pascal [log10(P) = A - (B / (T + C))]:, A=9.74022 (6.85941 for mm Hg), B=935.531,
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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				
3,110	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	ty Determi	nation	High	

^{*} Related References: 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. Vapor Pressure

OECD Harmonized

Template:

HERO ID: 5736675

FXTR	ACTION	

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 $300.05K = 297.9 \text{ kPa}$ and 297.6 kPa

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

Study Citation:		sion, (2012). 1,3-Butadiene [MAK value	documentation, 2	2001]. :51-70.
OECD Harmonized	Vapor Pressure			
Template: HERO ID:	9493518			
HERO ID.	9493316		EXTEN A CONTO	A.V
Danamatan		Data	EXTRACTIO	N
Parameter		Data		
Vapor Pressure		2477 - hPa		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and		no; not specified; Not Reported		
Solvent, Reactivity, Storag		Not Reported; Not Reported; Not Report	ted: Not Reported	
Radiolabel, Source, State,	•	Not Reported; Not Reported; Not Report	_	
Temperature	<i>y</i>	20 C	, portou	
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
Domain		Metric	EVALUATIO Rating	N Comments
Domain 1: Substance			Tuning	Commonia
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features
		11 1	6	(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 Reliabil	lity			
2. Test Render	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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.
				per remember of duties of 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 Quali	ty Determi	nation	High	

^{*} Related References: no references cited

Study Citation:		ology Program (NTP), (1993). NTP technical inhalation studies).	nical report on th	e toxicology and carcinogenesis studies of 1,3-butadiene (CAS no. 106-99-0) in
OECD Harmonized	Vapor Pressure			
Template:	vapor riessare			
HERO ID:	5160111			
			EXTRACTIO	N
Parameter		Data	LATIMACTIO	•
W. D		1000 11		
Vapor Pressure		1900 - mm Hg		
CASRN and Test Material		106-99-0; Not Reported	. 1	
Confidentiality, Type, and		Not Reported; Not Reported; Not Report		
Solvent, Reactivity, Storag		Not Reported; Not Reported; Not Report	_	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report 20 C	tea; Not Reported	
Temperature				
System Standard Deviation Results	0	Not Reported Not Reported		
Results Details	8	*		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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				
Domain 3. Outer	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	High	

^{*} Related References: 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: OECD Harmonized	NCBI, (2020). I Vapor Pressure	PubChem Compound Summary for CID	7845 1,3 Butadie	ne.
Template:	vapor i ressure			
HERO ID:	10171483			
	10171.00		EXTRACTIO	AT
Parameter		Data	EXTRACTIO	N
1 ai ainetei		Data		
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Repor	rted; Not Reported	
Temperature		Not Reported		
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Critical pressure 42.6 atm		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	tv Determi	nation	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: OECD Harmonized Template:	NCBI, (2020). Provide Vapor Pressure	ubChem Compound Summary for CID 7845 1,3 Butadiene.
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, Storag	e, and Stability	Not Reported; Not Reported; Not Reported
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Reported
Temperature		Not Reported
System		Not Reported
Standard Deviation Result	s	Not Reported
Results Details		Heat of Vaporization: 20.86 kJ/mol at 25 C; 22.47 kJ/mol at -4.41 C

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliab	oility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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.

^{*} 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: OECD Harmonized	NIOSH, (2007). NIOSH pocket guide to chemical hazards. Vapor Pressure
Template:	
HERO ID:	192177

HERO ID: 192177			
		EXTRACTIO	N .
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		
Геmperature	NR		
System	NR		
Standard Deviation Results	NR		
Results Details	Not Reported		
		EVALUATIO	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.

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

Study Citation: OECD Harmonized	NIOSH, (1992) Vapor Pressure	. Occupational safety and health guidelin	e for butadiene (1,3-butadiene).
Template: HERO ID:	8408503			
neko ib.	0400303		EXTRACTIO	N.
Parameter		Data	EATRACTIO	IN .
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, Storag	ge, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Report	ed; Not Reported	
Temperature		21 C (69.8 F)		
System		Not Reported		
Standard Deviation Result	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Quali	ty Determi	nation	High	

^{*} Related References: no references cited

Study Citation: OECD Harmonized Template:	NIST, (2022). N Vapor Pressure	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C		No; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	_	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ed; 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 f	rom the vapor pressure data reported by the method of least squares.
			EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance	36.1.1	D	*** 1	
	Metric 1:	Representativeness	High	Data 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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	v Dotormi	nation	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: OECD Harmonized Template:	NIST, (2022). N Vapor Pressure	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report		
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Report	ed; Not Reported	
Temperature		Not Reported		
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Enthalpy of Vaporization: 24.7 kJ/mol at	235 K	
			EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	tv Determi	nation	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: OECD Harmonized	NIST, (2022). NIST, Vapor Pressure	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
Template:				
HERO ID:	10225178			
			EXTRACTIO	N
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	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Temperature		Not Reported		
System		Not Reported		
Standard Deviation Results	3	Not Reported		
Results Details		Enthalpy of Vaporization: 21.1 kJ/mol		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	tv Determi	nation	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: OECD Harmonized	NIST, (2022). I Vapor Pressure	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
Template: HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		Not Reported		
Vapor Fressure CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guidalina	No; Experimental; Not Reported		
		Not Reported; Not Reported; Not Report	ted: Not Reported	
Solvent, Reactivity, Storage, and Stability Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Report		
Temperature		Not Reported	ica, rvoi reported	
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details	,	Enthalpy of Vaporization: 22.47 kJ/mol a	at 268.7 K	
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance			&	
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance 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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	tv Determi	nation	High	

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

Study Citation: OECD Harmonized	NIST, (2022). N Vapor Pressure	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.				
Template: HERO ID:	10225178							
HERO ID:								
Parameter		Data	EXTRACTIO	N				
1 ai ailletei		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	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported					
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Report	ted; Not Reported					
Temperature		Not Reported						
System		Not Reported						
Standard Deviation Results	S	Not Reported						
Results Details		0.08141 kJ/mol at 273.15 K, P=119.95 k	Pa					
			EVALUATIO	N				
Domain		Metric	Rating	Comments				
Domain 1: Substance								
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.				
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	lity							
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.				
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	ty Dotormi	nation	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, andvapor states, J. Res. NBS, 1945, 35, 39-85.

Study Citation: OECD Harmonized Template:	NIST, (2022). N Vapor Pressure	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and		No; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	_	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ed; 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 f	rom the vapor pressure data reported by the method of least squares.
			EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance		_		
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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.

^{*} 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: OECD Harmonized Template:	NIST, (2022). N Vapor Pressure	HST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	No; Experimental; Not Reported		
Solvent, Reactivity, Storage, and Stability		Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Report	ed; 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.
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabili	ty			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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.
		nation	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: OECD Harmonized Template:	NIST, (2022). N Vapor Pressure	IST Chemistry WebBook. 1,3-Butadieno	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and O		No; Experimental; Not Reported		
Solvent, Reactivity, Storage	-	Not Reported; Not Reported; Not Report	_	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Temperature		Not Reported		
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Enthalpy of Vaporization: 23.6 kJ/mol at	t 261 K.Calculated	from the vapor pressure data reported by the method of least squares.
			EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance	36.1.4		*** 1	
	Metric 1:	Representativeness	High	Data 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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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.
· · · · · · · · · · · · · · · · · · ·	·			

^{*} 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: OECD Harmonized Template:	NIST, (2022). N Vapor Pressure	VIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	No; Experimental; Not Reported		
Solvent, Reactivity, Storage	, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, a	nd Purity	Not Reported; Not Reported; Not Report	ed; 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.
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabili	ty			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Qualit	v Determi	nation	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: OECD Harmonized Template:	NIST, (2022). N Vapor Pressure	NIST Chemistry WebBook. 1,3-Butadieno	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		••
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C		No; Experimental; Not Reported		
Solvent, Reactivity, Storage	•	Not Reported; Not Reported; Not Report	•	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Temperature		Not Reported		
System Standard Deviation Results		Not Reported Not Reported		
Results Details		Enthalpy of vaporization: 21.47 kJ/mol		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance			8	
	Metric 1:	Representativeness	High	Data 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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	Dotomi	nation	High	

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

Study Citation: OECD Harmonized Template:	NIST, (2022). N Vapor Pressure	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		43.2 - bar		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	No; Experimental; Not Reported		
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, a		Not Reported; Not Reported; Not Report	_	
Temperature	•	Not Reported	•	
System		Not Reported		
Standard Deviation Results		1.0 bar		
Results Details		reported as critical vapor pressure.		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance			-	
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabili	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	v Determi	nation	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: OECD Harmonized Template:	NIST, (2022). N Vapor Pressure	TIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	ndard Reference Database No. 69.
HERO ID:	10225178			
			EXTRACTIO	N
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	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ted; 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	
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	ty Determi	nation	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: OECD Harmonized	NLM, (2003). I Vapor Pressure	PubChem: Hazardous Substance Data B	ank: 1,3-Butadien	e, 106-99-0.
Template:	, up of 11essure			
HERO ID:	5926134			
			EXTRACTIO	N
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, Storag		NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Temperature		25 C		
System		Not Reported		
Standard Deviation Result	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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.

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

Study Citation: OECD Harmonized	RSC, (2019). C Vapor Pressure	hemSpider: 1,3-Butadiene.		
Template:	-			
HERO ID:	5926255			
			EXTRACTIO	N
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, Storag	e, and Stability	NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Temperature	-	Not Reported		
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		2.4 atm		
Domain		Matria	EVALUATIO	
Domain Domain 1: Substance		Metric	Rating	Comments
Domain 1: Substance	Matria 1.	Dammagantativanaga	High	Determined an estimated for the militate hands of militate and
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that references a peer-reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.

^{*} Related References: NIOSH

Study Citation: OECD Harmonized	RSC, (2019). O Vapor Pressure	ChemSpider: 1,3-Butadiene.		
Template: 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		NR; NR; NR; NR		
Radiolabel, Source, State,		NR; NR; NR; NR		
Temperature	·	Not Reported		
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	tv Determi	ination	Medium	

^{*} Related References: SynQuest

Study Citation:
OECD Harmonized

Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.

DECD Harmonized Vapor Pressure

Template: HERO ID:

IERO ID: 5349186

		EXTRACTIO	NT
Parameter	Data	EATRACTIO	17
Noney Dragging	1012 mm Ha		
Vapor Pressure CASRN and Test Material	1912 mm Hg 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		
		EVALUATIO	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
Domain 3: Other			
Domain 3: Other Metric 5:	Databases	III.al-	Data in farma a managinal managinary di data a Nasakina
		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 Detern	nination	High	

Study Citation:	U.S. EPA, (1989	9). Health and environmental effects docu-	ment for 1,3-butadie	ne.
OECD Harmonized	Vapor Pressure			
Template:				
HERO ID:	3454			
			EXTRACTION	
Parameter		Data		
Vapor Pressure		1 - atm		
CASRN and Test Material		106-99-0; 1,3-butadiene		
Confidentiality, Type, and C	Guideline	No; Not specified; Not reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Reporte	ed; Not Reported	
Radiolabel, Source, State, a	nd Purity	Not Reported; Not Reported; Not Reporte	ed; 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 Reliabili	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	v Determi	nation	Medium	

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

Study Citation: OECD Harmonized	U.S. EPA, (1989) Vapor Pressure). Health and environmental effects docu	ument for 1,3-but	radiene.
Template:	1			
HERO ID:	3454			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Temperature		14.5°C		
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determir	nation	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.

Template: HERO ID: Parameter	3454	Data	EXTRACTIO	
Parameter		Doto	EVTDACTIO	
Parameter		Doto	EATRACTIO	N
		Data		
Vapor Pressure		5 - atm		
CASRN and Test Material		106-99-0; 1,3-butadiene		
Confidentiality, Type, and G		No; Not specified; Not reported		
Solvent, Reactivity, Storage,		Not Reported; Not Reported; Not Report	_	
Radiolabel, Source, State, ar	nd Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Temperature		47.0°C		
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance		_		
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.
Domain 2: Test Reliabili	.y			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	v Determin	etion	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: OECD Harmonized	U.S. EPA, (200 Vapor Pressure	2). Health assessment of 1,3-butadiene.		
Template:	1			
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	e, and Stability	NA; NA; NA; NA		
Radiolabel, Source, State, a	and Purity	NA; NA; gas; NA		
Temperature		20°C		
System		Not Reported		
Standard Deviation Results	S	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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	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 Qualit	ty Determi	nation	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: OECD Harmonized	U.S. EPA, (2019) Vapor Pressure	9). Chemistry Dashboard Information fo	r 1,3-Butadiene.	106-99-0
Template:	•			
HERO ID:	5926160			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		2110 mm Hg		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage	, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	nd Purity	NR; NR; NR; NR		
Temperature		Not Reported		
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that provides references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	v Determi	nation	High	

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

Study Citation: OECD Harmonized	U.S. EPA, (199 Vapor Pressure	6). Locating and estimating air emissions	from sources of	1,3-butadiene.
Template: HERO ID:	6389860			
			EXTRACTIO	N
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	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Temperature		15.3 C		
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabil	litv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Quali	ty Determi	nation	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 HERO ID: 69425)

Study Citation: OECD Harmonized	U.S. EPA, (1996) Vapor Pressure	6). Locating and estimating air emissions	s from sources of	1,3-butadiene.
Template: HERO ID:	6389860			
			EXTRACTIO	N
Parameter		Data		
Vapor Pressure		Not Reported		
CASRN and Test Material		106-99-0; 1,3-butadiene		
Confidentiality, Type, and C	Guideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Temperature		Not Reported		
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		critical pressure: 4.32 MPa (626 psi)		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	itv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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

^{*} 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 HERO ID: 69425)

Overall Quality Determination

Study Citation: OECD Harmonized Template:	U.S. EPA, (199 Vapor Pressure	6). Locating and estimating air emissions	from sources of	1,3-butadiene.
HERO ID:	6389860			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Temperature		Not Reported		
System		Not Reported		
Standard Deviation Results	S	Not Reported		
Results Details		Heat of vaporization389 J/g (93 cal/g) at	25 C418 J/g (100 d	cal/g) at bp
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Quali	tv Determi	nation	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 HERO ID: 69425)

Study Citation: OECD Harmonized	U.S. EPA, (199 Vapor Pressure	6). Locating and estimating air emissions	from sources of	1,3-butadiene.			
Template: 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, Storag		Not Reported; Not Reported; Not Report	ted; Not Reported				
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Report	ted; Not Reported				
Temperature		47.0 C					
System		Not Reported					
Standard Deviation Results		Not Reported					
Results Details		Not Reported					
			EVALUATIO	N .			
Domain		Metric	Rating	Comments			
Domain 1: Substance							
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.			
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabi	lity						
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.			
	Metric 4:	Reliability/Analytical Method	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 Quali	ty Determi	nation	High				

^{*} Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology,3rd ed, Volume 4. 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; Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID 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. logKow

OECD Harmonized

Template: HERO ID: 5155603

			EXTRACTIO	N
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, a	nd Stability	Not Reported; Not Reported; Not Repor	ted; Not Reported	
Radiolabel, Source, State, and	•	Not Reported; Not Reported; Not Repor	-	
Temperature	•	Not Reported		
System		Not Reported		
рH		Not Reported		
Results Details Method		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
1	Metric 1:	Representativeness	High	Data 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	Medium	There is no indication that the methodology for producing the information was biased
1		(Method Objectivity)	1.1caram	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	Determi	nation	High	

... continued from previous page

Study Citation: California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure

OECD Harmonized

level summaries. logKow

Template: HERO ID:

5155603

		EVALUATION		
Domain	Metric	Rating	Comments	

^{*} Related References: No source cited; extracted gray lit

Study Citation: OECD Harmonized Template:	EC, (2000). Pri logKow	iority Substances List Assessment Report:	: 1,3-Butadiene.			
HERO ID:	5160048					
			EXTRACTIO	N		
Parameter		Data				
log k _{ow}		1.99				
CASRN and Test Material		106-99-0; 1,3-Butadiene				
Confidentiality, Type, and		no; experimental; Not Reported				
Solvent, Reactivity, Storage, and Stability		Not Reported; Not Reported; Not Report				
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Report	ted; 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				
			EVALUATIO	N		
Domain		Metric	Rating	Comments		
Domain 1: Substance						
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.		
	Metric 2:	Appropriateness	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 Reliabi	litv					
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Quali	ty Determi	ination	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: OECD Harmonized Template:	ECB, (2002). I logKow	European Union risk assessment report: 1,	3-butadiene.				
HERO ID:	5155560						
			EXTRACTIO	N			
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 Report	ted; Not Reported				
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Report	ted; 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					
			EVALUATIO	N			
Domain		Metric	Rating	Comments			
Domain 1: Substance							
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.			
	Metric 2:	Appropriateness	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 Reliabi	litv						
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Quali	ty Determi	ination	High				

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

Study Citation: OECD Harmonized Template:	ECB, (2002). E logKow	European Union risk assessment report: 1,3-	-butadiene.	
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, Storag	e, and Stability	Not Reported; Not Reported; Not Reported	d; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Reported	d; 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 Reliabil	litv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	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.

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

Overall Quality Determination

Medium

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

OECD Harmonized Template:

logKow

Template: HERO ID:

5155560

EX1	rr.	4	\neg	rT(U.	N

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
Radiolabel, Source, State, and Purity	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 Reliab	bility							
	Metric 3:	Reliability/Unbiased	N/A	Rating of this factor is not applicable to this kind of information.				
		(Method Objectivity)						
	Metric 4:	Reliability/Analytical Method	N/A	Rating of this factor is not applicable to this kind of information.				
Domain 3: Other								
	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by 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: OECD Harmonized	ECB, (2002). E logKow	uropean Union risk assessment report: 1,3	3-butadiene.	
Template: HERO ID:	5155560			
HERO ID.	3133300		EXTRACTION	
Parameter		Data	EXTRACTION	
Tarameter		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, Storag		Not Reported; Not Reported; Not Reported	ed: Not Reported	
Radiolabel, Source, State, and Purity		Not Reported; Not Reported; Not Reported	•	
Temperature		Not Reported	· · · · · · · · · · · · · · · · · · ·	
System		Not Reported		
pН		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 Reliabil	lity			
Domain 2. Test Kenaon	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	medie 3.	(Method Objectivity)	Wicaram	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				
Bomain 3. Outer	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.
0 110 11	4 D 4		N. F. 11	
Overall Quali	ty Determi	nation	Medium	

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

Study Citation: OECD Harmonized Template:	Elsevier, (2019) logKow). Reaxys: physical-chemical property data	a for 1,3-butadie	ne. CAS Registry Number: 106-99-0
HERO ID:	5926412			
			EXTRACTIO	N
Parameter		Data		
log k _{ow}		1.902		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	and Purity	NR; NR; NR; NR		
Temperature		Not Reported		
System		Not Reported		
pН		Not Reported		
Results Details Method		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		1 data point was reported in Reaxys.		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
Metric 4:		(Method Objectivity) Reliability/Analytical Method	Medium	towards a particular product or outcome. Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
				and a contract of the contract
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a secondary database with a references to the peer-reviewed original source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit		4•	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	logKow

		EXTRACTIO	N
Parameter	Data		
lag k	1.9		
log k _{ow} CASRN and Test Material	1.9 106-99-0; 1,3-Butadiene		
Confidentiality, Type, and Guideline	None; Calculation; Not Reported		
Solvent, Reactivity, Storage, and Stability	NR; NR; NR		
Radiolabel, Source, State, and Purity	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-Softw	vare 1989	
		EVALUATION	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	Medium	Calculated data consistent with the subject chemical substance structural features.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased	High	The methodology for producing the information is designed to answer a specific ques-
	(Method Objectivity)	6 -	tion, 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
MEUIC O.	MODEIS	High	known.

Overall Quality Determination	High	

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

logKow

Template: HERO ID:

RO ID: 5932746

		EXTRACTIO	NI
Parameter	Data	EXTRACTIO	IN .
r ai ainetei	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	25°C		
System	Not Reported		
pH	Not Reported		
Results Details Method	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	Not Reported		
		EVALUATIO	N
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	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	Medium	There is no indication that the methodology for producing the information was biased
Wette 5.	(Method Objectivity)	Wediam	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 inclu-
	<u> </u>		sion 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.
1.10410 0.		- 1111	
Overall Quality Determi	ination	High	

Study Citation: OECD Harmonized Template:	U.S. EPA, (201 logKow	9). Chemistry Dashboard Information for	1,3-Butadiene.	106-99-0
HERO ID:	5926160			
			EXTRACTIO	N
Parameter		Data		
$\log k_{ow}$		1.99		
CASRN and Test Materia	1	106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storag	ge, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
Temperature		Not Reported		
System		Not Reported		
pН		Not Reported		
Results Details Method		Not Reported		
Standard Deviation Result	is	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabi	litv			
20 100 100 100 100 100 100 100 100 100 1	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	36.4	(Method Objectivity)	3.6.11	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: OECD Harmonized	U.S. EPA, (201 logKow	9). Chemistry Dashboard Information fo	or 1,3-Butadiene.	106-99-0
Template:	logitow			
HERO ID:	5926160			
			EXTRACTIO	N
Parameter		Data		
11-		1.99		
log k _{ow} CASRN and Test Material		1.99 106-99-0; 1,3-Butadiene		
	C! 1-1!	, ,		
Confidentiality, Type, and		None; Experimental; Not Reported NR; NR; NR; NR		
Solvent, Reactivity, Storag Radiolabel, Source, State,		NR; NR; NR; NR NR; NR; NR		
Temperature	and Furity	Not Reported		
System		Not Reported		
pH		Not Reported		
Results Details Method		Not Reported		
Standard Deviation Results	2	Not Reported		
Results Details	,	Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabil	lity			
Bomain 2. Test Remain	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	1.100110 01	(Method Objectivity)	1,10010111	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 inclu-
				sion 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 Quali	tv Determi	nation	High	
O / Clair Quan	ij Determi		111511	

^{*} Related References: PhysProp. Egon Willighagen

Study Citation: OECD Harmonized Template:	EC, (2000). Pri Water Solubility	ority Substances List Assessment Report: y	1,3-Butadiene.	
HERO ID:	5160048			
			EXTRACTIO	N
Parameter		Data		
Water Solubility		735 - mg/L		
CASRN and Test Material		106-99-0; Not Reported		
Confidentiality, Type, and C		no; experimental; Not Reported		
Solvent, Reactivity, Storage	-	Not Reported; Not Reported; Not Report		
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Temperature		25 C		
System		Not Reported		
рН		Not Reported		
Results Details Method		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		experimental at 25 C and 101.325 kPa		
ъ.		Mari	EVALUATIO	
Domain		Metric	Rating	Comments
Domain 1: Substance	Metric 1:	Representativeness	Uiah	Data and managed an actimated for the subject abording substance
	Metric 2:	Appropriateness	High Medium	Data are measured or estimated for the subject chemical substance. Data measured for a structural analogue of the subject chemical substance are consistent
	Metric 2.	Appropriateness	Medium	with what is expected for the subject chemical substance structural properties, features or behaviors.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit	ty Determi	nation	High	

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

Study Citation: OECD Harmonized	ECB, (2002). E Water Solubility	European Union risk assessment report: 1, y	3-butadiene.	
Template: HERO ID:	5155560			
			EXTRACTIO	N
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	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
Temperature		Not Reported		
System		Not Reported		
pН		Not Reported		
Results Details Method		gas-liquid chromatography		
Standard Deviation Results	;	Not Reported		
Results Details		(McAuliffe 1966)		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance			-	
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties
Domain 2: Test Reliabil	ity			
	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.

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

High

Overall Quality Determination

Study Citation:
OECD Harmonized

Mueller, M., Klein, W. (1992). Comparative evaluation of methods predicting water solubility for organic compounds. Chemosphere 25(6):769-782.

Water Solubility

		EXTRACTIO	N
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 partiti	on coefficients	
pH	Not reported	on coefficients.	
Results Details Method	Not Reported		
Standard Deviation Results	Not Reported		
Results Details	Reported as 1.36E-2 mol/L		
	r		
		EVALUATION	
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	High	The methodology for producing the information is designed to answer a specific ques-
	(Method Objectivity)	C	tion, 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
			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.

Study Citation: OECD Harmonized	NLM, (2003). Water Solubilit	PubChem: Hazardous Substance Data Ba	nk: 1,3-Butadien	e, 106-99-0.
	water Solubilit	У		
Template: HERO ID:	5926134			
неко ір:	3920134			
			EXTRACTIO	N
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, Storag		NR; NR; NR		
Radiolabel, Source, State,		NR; NR; NR; NR		
Temperature	•	20°C		
System		Not Reported		
рH		Not reported		
Results Details Method		Not Reported		
Standard Deviation Result	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliabi	lity			
Domain 2. Test Renaul	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available database that provides references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
0	4 D-4 '	2		~
Overall Quali	ty Determi	nation	High	

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

Study Citation: OECD Harmonized	RSC, (2019). Che Water Solubility	emSpider: 1,3-Butadiene.		
Template:				
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, Storag	e, 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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a 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 Quali	tv Determin	ation	Uninformative	

^{*} Related References: NIOSH

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

Template:

HERO ID: 5932745

		EXTRACTIO	N .
Parameter	Data		
Water Solubility	722 mg/I		
CASRN and Test Material	733 mg/L 106-99-0; 1,3-Butadiene		
	* *		
Confidentiality, Type, and Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage, and Stability Radiolabel, Source, State, and Purity	NR; NR; NR; NR NR; NR; NR; NR		
	25°C		
Temperature			
System	Not Reported		
pH	Not reported	.: 1 (101.22	51D (1 () ' ''' ''' ' '' 1 () O ' ' 1 () 0 725 / H20
Results Details Method	converted using CRC handbook's re		5 kPa (1 atm) in equilibrium with the solution. Originally reported as 0.735 g/kg H20,
Standard Deviation Results	Not Reported	eported water density at	25 C.
Results Details	Not Reported		
		EVALUATIO	N.
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
			, , , , , , , , , , , , , , , , , , ,
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	(Method Objectivity)		towards a particular product or outcome.

Overall Quality Determination		High		
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 5:	Databases	High	Data is from a peer-reviewed data collection.
Domain 3: Other				
	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.
	3.5	(Method Objectivity)	3.6.11	towards a particular product or outcome.
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
Domain 2: Test Relia	ability			

Study Citation: OECD Harmonized	U.S. EPA, (2002 Water Solubility	2). Health assessment of 1,3-butadiene.		
Template:				
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	e, and Stability	NR; NR; NA; NA		
Radiolabel, Source, State, a	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 Reliabil	:+			
Domain 2. Test Kenaon	Metric 3:	Reliability/Unbiased	N/A	Detine of this featon is not applicable to this kind of information
	Metric 3.	(Method Objectivity)	IV/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
	Wictire 4.	Renability// marytical Method	Wediam	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.

^{*} 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.

U.S. EPA, (2019). Chemistry Dashboard Information for 1,3-Butadiene. 106-99-0..

OECD Harmonized	Water Solubility	Ž	,	
Template: HERO ID:	5926160			
HERO ID.	3920100		EVED A CETO	NAT.
Parameter		Data	EXTRACTIO	ON .
		244		
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, Storag	ge, 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 Result	S	Not Reported		
Results Details		Reported as 1.36E-2 mol/L		
			EVALUATIO	N .
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.

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

^{*} Related References: PhysProp. McAuliffe, C 1966

Study Citation:

Study Citation:		California Office of Environmental Health Hazard Assessment :: OEHHA (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure				
OECD Harmonized	level summarie Flash Point	S.				
Template:						
HERO ID:	5155603					
			EXTRACTIO	N		
Parameter		Data				
Flash Point		-76 C				
CASRN and Test Material	1	106-99-0; 1,3-butadiene				
Confidentiality, Type, and		No; Not specified; Not Reported				
Solvent, Reactivity, Storag		Not Reported; Not Reported; Not Report	ted: Not Reported			
Radiolabel, Source, State,		Not Reported; Not Reported; Not Report				
System		Not Reported	,			
Standard Deviation Result	is	Not Reported				
Results Details		Not Reported				
			EVALUATIO	Ai		
Domain		Metric	Rating	Comments		
Domain 1: Substance			&			
	Metric 1:	Representativeness	High	Data 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.		
D ' 2 T (D 1' 1 '	1'.					
Domain 2: Test Reliabi	Metric 3:	Daliahility/Hahiagad	Madia			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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						
Domain 5. Onici	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are		
	Medic 3.	Damouses	mgn	peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.		
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.		
Overall Quali	ty Determi	nation	High			
Overan Quan	ty Determine	เมลมปม	mgir			

^{*} Related References: No source cited; extracted gray lit

Study Citation: OECD Harmonized	Coleman, R. S., Flash Point	, Alegria, H. A. (2001). 1,3-Butadiene. :1	-4.	
Template: HERO ID:	9493522			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
System		Not Reported		
Standard Deviation Results	3	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical 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 Reliabil	litv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Quali	ty Determi	nation	High	

^{*} Related References: no references cited

Study Citation: OECD Harmonized Template:	ECB, (2002). E Flash Point	uropean Union risk assessment report: 1	,3-butadiene.	
HERO ID:	5155560			
			EXTRACTIO	N
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	e, and Stability	Not Reported; Not Reported; Not Repor	ted; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Repor	ted; Not Reported	
System		Closed Cup		
Standard Deviation Results		Not Reported		
Results Details		DIN 51755, Sax and Lewis, 1987		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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

HERO ID: 5155560 Table: 1 of 1

^{*} 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: OECD Harmonized	Grub, J., Löser, Flash Point	E. (2011). Butadiene. :381-396.		
Template: HERO ID:	9493526			
			EXTRACTIO	N
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	e, and Stability	Not Reported; Not Reported; Not Reported	ed; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Reported	ed; Not Reported	
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (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 Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qualit			High	

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

Study Citation: OECD Harmonized	Kerns, M., Henr Flash Point	ning, S., Rachita, M. (2002). Butadiene p	polymers. :317-35	56.
Template: HERO ID:	9493542			
			EXTRACTIO	N
Parameter		Data		
Flash Point		761 6		
CASRN and Test Material		-76.1 - C 109-66-0; 1,3-Butadiene		
Confidentiality, Type, and	Cuidalina	no; not specified; Not Reported		
Solvent, Reactivity, Storage		Not Reported; Not Reported; Not Report	tad: Not Paportad	
Radiolabel, Source, State,		Not Reported; Not Reported; Not Report	•	
System	and I unity	Not Reported	ica, rvoi reportea	
Standard Deviation Results		Not Reported		
Results Details	,	Not Reported		
			EVALUATIO	N.
Domain		Metric	Rating	Comments
Domain 1: Substance			<u> </u>	
	Metric 1:	Representativeness	High	Data 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 Reliabil	itv			
2. 1000 100000	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Quali	tv Determi	nation	High	

HERO ID: 9493542 Table: 1 of 1

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

Study Citation: OECD Harmonized	NIOSH, (2007) Flash Point	. NIOSH pocket guide to chemical haza	rds.	
Template: HERO ID:	192177			
			EXTRACTIO	N
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		NR; NR; NR		
Radiolabel, Source, State, a		NR; NR; Liquid; NR Notes: NR		
System	Ž	closed cup		
Standard Deviation Results	3	NR		
Results Details		NR		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	itv			
	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.

High

Overall Quality Determination

Study Citation: OECD Harmonized	NIOSH, (1992) Flash Point	. Occupational safety and health guideling	ne for butadiene (1,3-butadiene).
Template: HERO ID:	8408503			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	rted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	rted; Not Reported	
System		Not Reported		
Standard Deviation Results	s	Not Reported		
Results Details		also report 105 C		
			EVALUATIO:	N N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Reliabil	litv			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that 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 Quali	ty Determi	nation	High	

^{*} Related References: no references cited

Study Citation: OECD Harmonized	RSC, (2019). C Flash Point	ChemSpider: 1,3-Butadiene.		
Template: HERO ID:	5926255			
			EXTRACTIO	N
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, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
System		Not Reported		
Standard Deviation Results	S	Not reported		
Results Details		-105°F (-76.1111°C) (Gas, Liquid, None))	
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
		(Method Objectivity)		towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is unknown but is likely to be 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: OECD Harmonized Template:	RSC, (2019). C Flash Point	ChemSpider: 1,3-Butadiene.		
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	e, and Stability	NR; NR; NR		
Radiolabel, Source, State, a	and Purity	NR; NR; NR; NR		
System		Not Reported		
Standard Deviation Results	3	Not reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	tv Determi	nation	Medium	

^{*} Related References: Oxford University Chemical Safety Data

Study Citation: OECD Harmonized	RSC, (2019). C Flash Point	ChemSpider: 1,3-Butadiene.		
Template: 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, Storag		NR; NR; NR		
Radiolabel, Source, State,	-	NR; NR; NR; NR		
System	-	Not Reported		
Standard Deviation Results	s	Not reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	tv Determi	ination	Medium	

^{*} Related References: SynQuest

Study Citation: OECD Harmonized	RSC, (2019). C	ChemSpider: 1,3-Butadiene.		
	riasn Point			
Template: HERO ID:	5926255			
HERO ID;	J7202JJ			
_		. .	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		NR; NR; NR		
Radiolabel, Source, State,	•	NR; NR; NR		
System	and I arrey	Not Reported		
Standard Deviation Results	S	Not reported		
Results Details		Not Reported		
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	M	(Method Objectivity)	T	towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
Domain J. Ouici	Metric 5:	Databases	High	Data is from a publicly available database that provides references to the original, peer-
	menic J.	Databases	IIIgii	reviewed source.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
0 110 11	4 D 4 9		N. J.	
Overall Quality	ty Determi	ination	Medium	

^{*} Related References: Sigma-Aldrich

Study Citation: OECD Harmonized	U.S. EPA, (200 Flash Point	2). Health assessment of 1,3-butadiene.		
Template: HERO ID:	52152			
HERO ID:	52153			
D 4		D . (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, Storag		NA; NA; NA		
Radiolabel, Source, State,	•	NA; NA; gas; NA		
System	·	NA		
Standard Deviation Results	S	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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.
Domain 3: Other				
	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	tv Determi	nation	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: OECD Harmonized	U.S. EPA, (1996 Flash Point	6). Locating and estimating air emission	ns from sources of	1,3-butadiene.
Template:	(2000/0			
HERO ID:	6389860			
			EXTRACTIO	N
Parameter		Data		
Flash Point		-105 - C		
CASRN and Test Material		106-99-0; 1,3-butadiene		
Confidentiality, Type, and		no; not specified; Not Reported		
Solvent, Reactivity, Storag		Not Reported; Not Reported; Not Repo	orted: Not Reported	
Radiolabel, Source, State,	•	Not Reported; Not Reported; Not Reported	•	
System		Not Reported	· · · · · · · · · · · · · · · · · · ·	
Standard Deviation Results	S	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance			8	
	Metric 1:	Representativeness	High	Data 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 Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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				
Domain 3. Outer	Metric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	ty Determi	nation	High	

^{*} Related References: source vaguely references both Kirshenbaum, I. Butadiene. In: Kirk-Othmer Encyclopedia of Chemical Technology,3rd ed, Volume 4. 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; Van Nostrand Reinhold Company, Inc., 1981. p. 177. (HERO ID HERO ID: 69425)

Study Citation: OECD Harmonized	ECB, (2002). E Autoflammabil	European Union risk assessment report: 1, ity	3-butadiene.	
Template: HERO ID:	5155560			
			EXTRACTIO	N
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, Storag	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,	and Purity	Not Reported; Not Reported; Not Report	ted; Not Reported	
System		Not Reported		
Standard Deviation Result	S	Not Reported		
Results Details		reference to DIN 51794		
Results Value		Not Reported		
			EVALUATIO	N .
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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.

^{*} Related References: cited from BASF safety data sheet

Study Citation: OECD Harmonized Template:	ECB, (2002). E Autoflammabili	European Union risk assessment report: 1, ity	3-butadiene.	
HERO ID:	5155560			
			EXTRACTIO	N
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	e, and Stability	Not Reported; Not Reported; Not Report	ted; Not Reported	
Radiolabel, Source, State,		Not Reported; Not Reported; Not Report	ted; Not Reported	
System		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
Results Value		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	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 Over	tv. Dotomos:	nation	High	
Overall Quality	iy Deterim	แลนบแ	High	

^{*} Related References: cited from Auer (1989). Auer-Technikum, Ausgabe 12, Auer-Gesellschaft mbH, Berlin, 146-151. andHommel G (1987). Handbuch der gefaehrlichen Gueter, Merkblatt 44, 4 neubearbeitete Auflage, Springer Verlag,Berlin.

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

Template:

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

Study Citation:
OECD Harmonized

Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.

Autoflammability

Template: HERO ID:

			EXTRACTIO	N
Parameter		Data		
Auto-flammability		420 C		
CASRN and Test Material	l	106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guideline	None; Experimental; Not specified		
Solvent, Reactivity, Storag		NR; NR; NR		
Radiolabel, Source, State,	and Purity	NR; NR; NR; NR		
System	•	Not reported		
Standard Deviation Result	S	Not Reported		
Results Details		Not Reported		
Results Value		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabi	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	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 Quali	tv Determi	nation	High	

Study Citation:
OECD Harmonized

Sun, H. N., Wristers, J. P. (2002). Butadiene.

Autoflammability

Template: HERO ID:

HERO ID: 5349	9218						
			EXTRACTIO	N			
Parameter		Data					
Auto Governalilles		417.9 C					
Auto-flammability CASRN and Test Material		417.8 - C 106-99-0: 1.3-Butadiene					
		, ,					
Confidentiality, Type, and Guideline		no; not specifed; Not Reported Not Reported; Not Reported; Not Reported					
Solvent, Reactivity, Storage, and S Radiolabel, Source, State, and Pur		Not Reported; Not Reported; Not Reported	_				
System	пу	Not Reported Not Reported	ied, Not Reported				
Standard Deviation Results		Not Reported					
Results Details		Not Reported					
Results Value		Not Reported					
Results value		Not Reported					
			EVALUATIO	N			
Domain		Metric	Rating	Comments			
Domain 1: Substance							
Met	ric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.			
Met	ric 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.			
				of defiaviors.			
Domain 2: Test Reliability							
•	ric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased			
		(Method Objectivity)		towards a particular product or outcome.			
Met	ric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate OR the analyti-			
				cal method is unknown but is likely to be appropriate based on the data's inclusion in a			
				peer-reviewed/recognized database or other secondary source.			
Domain 3: Other							
	ric 5:	Databases	High	The information or data is from a recognized data collection/repository where data are			
Wiet	11C J.	Databases	mgn	peer-reviewed by experts in the field, are broadly available to the public for review and			
				use OR includes references to the original sources.			
Met	ric 6:	Models	N/A	Rating of this factor is not applicable to this kind of informatio			
Overall Ossalitas D	\0.40r	matian	TT! ~1-				
Overall Quality D	etermi	กลนงก	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: OECD Harmonized	Grub, J., Löser, Viscosity	E. (2011). Butadiene. :381-396.		
Template:	Viscosity			
HERO ID:	9493526			
			EXTRACTIO	N
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	e, and Stability	Not Reported; Not Reported; Not Report	ed; Not Reported	
Radiolabel, Source, State, a	and Purity	Not Reported; Not Reported; Not Report	ed; Not Reported	
Temperature		50 C		
Test Conditions		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	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 Reliabil	ity			
	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.

^{*} 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: OECD Harmonized	Grub, J., Löser, Viscosity	E. (2011). Butadiene. :381-396.		
Template: HERO ID:	9493526			
			EXTRACTIO	N
Parameter		Data		
Viscosity		0.25 -		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	duideline	no; not specified; Not Reported		
Solvent, Reactivity, Storage	, and Stability	Not Reported; Not Reported; Not Reported	rted; Not Reported	
Radiolabel, Source, State, a	nd Purity	Not Reported; Not Reported; Not Repo	rted; Not Reported	
Temperature		25 C		
Test Conditions		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	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 Reliabili	ty			
	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 Qualit	v Determi	nation	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: OECD Harmonized	NLM, (2003). I Viscosity	PubChem: Hazardous Substance Data Ba	nk: 1,3-Butadien	e, 106-99-0.
Template: HERO ID:	5926134			
			EXTRACTIO	N
Parameter		Data		
Viscosity		0.00754		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and C	Guideline	None; Experimental; Not reported		
Solvent, Reactivity, Storage	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State, a	and Purity	NR; NR; NR; NR		
Temperature		20°C		
Test Conditions		Not Reported		
Standard Deviation Results		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qualit	ty Determi	nation	High	

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

Study Citation: OECD Harmonized	NLM, (2003). I Viscosity	PubChem: Hazardous Substance Data Ba	nk: 1,3-Butadien	e, 106-99-0.
Template: HERO ID:	5926134			
			EXTRACTIO	N
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	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,	-	NR; NR; NR; NR		
Temperature		-40°C		
Test Conditions		Not Reported		
Standard Deviation Results	s	Not Reported		
Results Details		Not Reported		
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	lity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 3: Other				
	Metric 5:	Databases	High	Data is from a publicly available, peer-reviewed database that provides references to a recognized data collection.
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quali	tv Determi	nation	High	

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

Study Citation: OECD Harmonized	Elsevier, (2019). Refractive Index	. Reaxys: physical-chemical property dat	a for 1,3-butadie	ene. CAS Registry Number: 106-99-0			
Template:							
HERO ID:	5926412						
			EXTRACTIO	N			
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, Storag		NR; NR; NR; NR					
Radiolabel, Source, State,	•	NR; NR; NR; NR					
Temperature		20°C					
System		Not Reported					
Standard Deviation Result	S	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					
			EVALUATIO	N			
Domain		Metric	Rating	Comments			
Domain 1: Substance							
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.			
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.			
Domain 2: Test Reliabi	lity						
	•	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased			
	Metric 3:						
	Metric 3:	(Method Objectivity)		towards a particular product or outcome.			

* Related References: Data point includes multiple primary sources in REAXYS	* Related References:	Data point include	s multiple primary	sources in REAXYS
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Databases

Models

Metric 5:

Metric 6:

Overall Quality Determination

Domain 3: Other

High

N/A

High

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

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

Study Citation:	O'Neil, M. J. (2013). 1,3-Butadiene. 106-99-0. :267.
OECD Harmonized	Refractive Index

Template:

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

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

^{*} Related References: Parchem-fine & specialty chemicals

Study Citation:
OECD Harmonized

Rumble, J. R., (Ed.) (2018). 1,3-Butadiene. :3-8.

Refractive Index

Template: HERO ID:

		EXTRACTIO	N
Parameter	Data	EXTRACTIO	•
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		
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		
		EVALUATIO	
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
	(Method Objectivity)		towards a particular product or outcome.
Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclu-
			sion 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.
0 110 12 D 4	• 4•	TT. 1	
Overall Quality Determ	ination	High	

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

Template:

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				
Solvent, Reactivity, Storage, and Stability	Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, and Purity	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			

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	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 Relial	bility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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 Qual	lity Determ	ination	High	

^{*} Related References: cited from Mackay, D. and W.Y. Shiu. 1981. A criticalreview of Henry's law constants for chemicalsof environmental interest. J. Phys. Chem. Ref.Data 10: 1175–1199.

Study Citation:	NCBI, (2020). PubChem	Compound Summary	for CID 7845 1,3 Butadiene.
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OECD Harmonized

Henry's Law

Template:

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			
Radiolabel, Source, State, and Purity	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			

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance	;			
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (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 Relia	bility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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.

	•		
continued	from	previous	page

Study Citation: NCBI, (2020). PubChem Compound Summary for CID 7845 1,3 Butadiene. Henry's Law

Template:

HERO ID: 10171483

		EVALUATION		
Domain	Metric	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: OECD Harmonized	NIST, (2022). N Henry's Law	NIST Chemistry WebBook. 1,3-Butadiene	e (106-99-0). Sta	andard Reference Database No. 69.		
Template: HERO ID:	10225178					
			EXTRACTIO)N		
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, Storag		Not Reported; Not Reported; Not Report	ted; Not Reported			
Radiolabel, Source, State,		Not Reported; Not Reported; Not Report	_			
Temperature	·	Not Reported	-			
рН		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 citat	tion and doesn't se	em well documented.		
Results Details Methods		Not Reported				
			EVALUATIO	N		
Domain		Metric	Rating	Comments		
Domain 1: Substance						
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.		
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.		
Domain 2: Test Reliabi	lity					
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.		
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.		
D : 2 04						
Domain 3: Other						

Metric 5:

Metric 6:

Overall Quality Determination

Databases

Models

N/A

Low

original sources.

Medium The data are from a source that is known but is missing elements required for High

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

designation such as peer-review, public availability, or the inclusion of references to

^{*} Related References: missing citation

Study Citation:	Rumble, J. R. (2018). Aqueous solub	ility and Henry's law constants of or	ganic compounds. :5-148 - 5-177.
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OECD Harmonized

Henry's Law

Template:

		EXTRACTIO	N
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 (converte	ed using $1 \text{ kPa} = 0$.	.00986923 atm)
Results Details Methods	Not Reported		
		EVALUATIO	N .
Domain	Metric	Rating	Comments
Domain 1: Substance			
Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.
Domain 2: Test Reliability			
Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased
Medic 3.	remaining, enclased	1,10didiii	There is no material that the methodology for producing the information was blased

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

Study Citation: OECD Harmonized	U.S. EPA, (198 Henry's Law	9). Health and environmental effects docur	ment for 1,3-butadien	ne.		
Template:	Ticiny 5 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		Not Reported; Not Reported; Not Reporte	d; Not Reported			
Radiolabel, Source, State,		Not Reported; Not Reported; Not Reporte	-			
Temperature	•	25°C				
pH		Not Reported				
System		Not Reported				
Standard Deviation Results	S	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 Reliabil	itv					
Domain 2. Test Kellauli	Metric 3:	Reliability/Unbiased	Medium	There is no indication that the methodology for producing the information was biased		
	monie 5.	(Method Objectivity)	Modfalli	towards a particular product or outcome.		
	Metric 4:	Reliability/Analytical Method	Low	The analytical method is unknown and there is no indication that a reliable method was used.		
Domain 3: Other						
Domain J. Other	Metric 5:	Databases	Medium	The data are from a source that is known but is missing elements required for High		
	wienie J.	Databases	Mediulli	designation such as peer-review, public availability, or the inclusion of references to original sources.		
	Metric 6:	Models	N/A	Rating of this factor is not applicable to this kind of information.		
Overall Quali	ty Determi	nation	Medium			

^{*} Related References: 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: OECD Harmonized Template:	Rumble, J. R., (Dielectric Cons	Ed.) (2018). 1,3-Butadiene. :3-8. tant		
HERO ID:	5349186			
			EXTRACTIO	N
Parameter		Data		
CASRN and Test Material		106-99-0; 1,3-Butadiene		
Confidentiality, Type, and	Guideline	None; Experimental; Not Reported		
Solvent, Reactivity, Storag	e, and Stability	NR; NR; NR; NR		
Radiolabel, Source, State,		NR; NR; NR; NR		
Dielectric Constant	·	2.050		
Temperature		Not Reported		
System		Not Reported		
Results Value		Not Reported		
Results Details		Not Reported		
			EVALUATIO	N N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	N/A	Rating of this factor is not applicable to this kind of information.
Domain 2: Test Reliabil	ity			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognize d database or other secondary source.

Overall Quality Determination	High
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Databases

Models

Metric 5:

Metric 6:

High

N/A

Data is from a recognized, peer-reviewed data collection.

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

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

onized UV and Visible Absorption

Template:

Parameter

Results Details

HERO ID: 5160048

	EXTRACTION
Data	

insignificant above 230 nm

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
Radiolabel, Source, State, and Purity	Not Reported; Not Reported; Not Reported
Wave Length Range	230 nm
Light Source, Optical Path Length, and Optical	Not Reported; Not Reported
Cell Type	
Test Concentration and Reference Substance	Not Reported; Not Reported
Solvent and Solvent pH	Not Reported; Not Reported
Blank Control, Maxima, Lambda Max, and Peak	Not Reported; Not Reported; Not Reported
Band Width	
Measured Absolute Value and Molar Coefficient	Not Reported; Not Reported

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	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 Relial	bility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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.

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

Template:

UV and Visible Absorption

HERO ID:

HERO ID: 5100	7040		
		EVALUATION	
Domain	Metric	Rating	Comments
Overall Quality Determination		High	
-			

^{*} Related References: cited from Jaber, H.M., W.R. Mabey, A.T. Liu, T.W. Chouand H.L. Johnson. 1984. Data acquisition forenvironmental 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-

OECD Harmonized

731. UV and Visible Absorption

Template:

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		
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;		
Cell Type	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	Not Reported; Not Reported; aprox. 210 based on figure 1; 160-240 nm		
Band Width Measured Absolute Value and Molar Coefficient	Not Reported; Not Reported		
Results Details	measured at 333 K, 313 K, 295 K, 273 K, 253 K, and 218 K		
Trooping Demand	110 100 100 100 100 100 100 100 100 100		

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Substance				
	Metric 1:	Representativeness	High	Data are measured or estimated for the subject chemical substance.
	Metric 2:	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties
Domain 2: Test Reliab	bility			
	Metric 3:	Reliability/Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.
	Metric 4:	Reliability/Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate 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.

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. UV and Visible Absorption **OECD Harmonized**

Template: HERO ID:

5621443

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

^{*} Related References: no references cited

Study Citation: OECD Harmonized Sun, H. N., Wristers, J. P. (2002). Butadiene.

UV and Visible Absorption

Template:

HERO ID: 5349218

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
Radiolabel, Source, State, and Purity	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

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

Overall Quality Determination High

Study Citation: OECD Harmonized Sun, H. N., Wristers, J. P. (2002). Butadiene.

UV and Visible Absorption

Template:

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 ⋅ m³/mol	Atmospheres - cubic meters per mole	
C	Celsius	
CASRN	Chemical Abstract Service registry number	
cP	Centipoise	
CRC	CRC Handbook of Chemistry and Physics	
DOE	U.S. Department of Energy	
ECB	European Chemicals Bureau	
EPA	Environmental Protection Agency	
F	Fahrenheit	
GC	Gas Chromatography	
g/cm ³	Grams per cubic centimeter	
GLP	Good Laboratory Practice	
HLC	Henry's Law Constant	
HPV	High Production Volume	
HSDB	Hazard Substance Data Bank	
ILO	International Labour Organization	
IPCS	International Programme on Chemical Safety	
IUCLID	International Uniform Chemical Information Database	
K	Kelvin	
Koa	Octanol-Air partition coefficient	
Kow	Octanol-Water partition coefficient	
mg/L	Milligrams per Liter	
mol	Mole	
mmHg	Millimeters of Mercury	
MS	Mass Spectrometry	
N/A	Not Applicable	
NICNAS	National Industrial Chemicals Notification and Assessment Scheme	
NLM	National Library of Medicine	
NR	Not Reported	
OECD	Organisation for Economic Co-operation and Development	
Pa (hPa)	Pascals (hectopascals; 1 hPa = 100 Pa)	
pH	Negative base 10 Log of Hydrogen Ion (H+) Concentration in Aque-	
	ous Solution	
pKa	Negative base 10 Log of Acid Dissociation Constant (Ka)	
RIVM	National Institute for Public Health and the Environment (Dutch: Ri-	
	jksinstituut voor Volksgezondheid en Milieu)	

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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