

Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport 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.

Table of Contents

HERO ID	Reference	Page
Photolysis in Air		
5705275	Andersson, Y., Ljungstrom, E. (1967). Gas phase reaction of the NO3 radical with organic compounds in the dark. Atmospheric Environment 23(5):1153-1155.	5
5675250	Andersson, Y., Ljungström, E. (1989). Gas phase reaction of the NO3 radical with organic compounds in the dark. Atmospheric Environment (1967) 23(5):1153-1155.	8
7348613	EC, (2002). Summary risk assessment report for 1,3-butadiene.	10
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	14
860294	Ghosh, B., Bugarin, A., Connell, B. T., North, S. W. (2010). OH radical initiated oxidation of 1,3-butadiene: isomeric selective study of the dominant addition channel. Journal of Physical Chemistry A 114(16):5299-5305.	38
5696791	Greenwald, E. E., Park, J., Anderson, K. C., Kim, H., Reich, B. J., Miller, S. A., Zhang, R., North, S. W. (2005). The OH-initiated oxidation of 1,3-butadiene in the presence of O2 and NO: a photolytic route to study isomeric selective reactivity. DUPE - Journal of Physical Chemistry A 109(35):7915-7922.	40
11779754	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.	42
1696190	Jenkin, M. E., Boyd, A. A., Lesclaux, R. (1998). Peroxy radical kinetics resulting from the OH-Initiated oxidation of 1,3-butadiene, 2,3-dimethyl-1,3-butadiene and isoprene. Journal of Atmospheric Chemistry 29(3):267-298.	47
5618698	Khaled, F., Giri, B. R., Liu, D., Assaf, E., Fittschen, C., Farooq, A. (2019). Insights into the Reactions of Hydroxyl Radical with Diolefins from Atmospheric to Combustion Environments. Journal of Physical Chemistry A 123(11):2261-2271.	49
660158	Klamt, A. (1993). Estimation of gas-phase hydroxyl radical rate constants of organic compounds from molecular orbital calculations. Chemosphere 26(7):1273-1289.	51
598253	Liu, X., Jeffries, H. E., Sexton, K. G. (1999). Hydroxyl radical and ozone initiated photochemical reactions of 1,3-butadiene. Atmospheric Environment 33(18):3005-3022.	53
3254900	Orlando, J. J., Tyndall, G. S., Apel, E. C., Riemer, D. D., Paulson, S. E. (2003). Rate coefficients and mechanisms of the reaction of Clatoms with a series of unsaturated hydrocarbons under atmospheric conditions. International Journal of Chemical Kinetics 35(8):334-353.	55
5589165	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.	57
618974	Sexton, K. G., Doyle, M. L., Jeffries, H. E., Ebersviller, S. (2007). Development and testing of a chemical mechanism for atmospheric photochemical transformations of 1,3-butadiene. Chemico-Biological Interactions 166(1-3):156-162.	69
1742345	Tuazon, E. C., Alvarado, A., Aschmann, S. M., Atkinson, R., Arey, J. (1999). Products of the gas-phase reactions of 1,3-butadiene with OH and NO3 radicals. Environmental Science & Technology 33(20):3586-3595.	72
3454	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.	76
5699949	Vimal, D. (2008). Laboratory investigations of the hydroxyl radical-initiated oxidation of atmospheric volatile organic compounds. Pro- Quest Dissertations and Theses Doctoral Dissertation:213.	80
Hydrolysis		
6628926	NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.	83

Table of Contents

1,3-Butadiene

11779754	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.	85
Photolysis in Soil		
Biodegradation in Water		
11779754	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.	87
6628926	NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.	95
Biodegradation in Sediment		
Biodegradation in Soil		
11779754	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381.	99
Aquatic Bioconcentration	1,5 building: 1500 501.	
Terrestrial Bioconcentration		
Adsorption and Desorption		
Miscellaneous		
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	101
901429	Zhao, Z., Husainy, S., Smith, G. D. (2011). Kinetics studies of the gas-phase reactions of NO3 radicals with series of 1-alkenes, dienes, cycloalkenes, alkenols, and alkenals. Journal of Physical Chemistry A 115(44):12161-12172.	107
Other Properties		
List of Abbreviations and Acronyms fo	or Data Quality Evaluation and Extraction Tables	109

Study Citation: Andersson, Y., Ljungstrom, E. (1967). Gas phase reaction of the NO3 radical with organic compounds in the dark. Atmospheric Environment 23(5):1153-

OECD Harmonized

Photolysis in Air

Template:

HERO ID: 5705275

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EXTR	Δι	"	111	1	N

	EXTRACTION			
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, Guideline	None; Experimental; other: Gas phase reaction of the NO3 radical with organic compounds			
Solvent, Reactivity, Storage, Stability	NR; NR; NR			
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR			
Duration and Test Temperature	data collected over 30 minutes; 296±1K			
Light Source, Intensity, and additional light de-	Dark; Not applicable; Not applicable			
tails Source Wavelength Lower and Upper	Not applicable; Not applicable			
Test Details and Control	N2O5 was source of the NO3 radical; Not reported			
Initial Concentration, Reference	10-600 ppm; Not reported			
Compound				
Substance Wavelength Lower and Upper	Not applicable; Not applicable			

4.4±0.8E-14 cm3/molecule.sec; Nitrate radical reaction rate

Direct Quantum Yield Results, Direct Half Life

by Loss Lower and Upper

Indirect Type Results, Indirect Rate Constant Lower and Upper

Method Details Results and Products

Details Results

Parameter Value and Parameter Results Reference Substance Results, Percent Degrada-

tion Results and Standard **Deviation Results**

Results Remarks, Sample time Results, Results Details

Not reported; Not reported

Not reported; Not reported; Not reported

Not reported; Not reported

Not reported; Not reported; Not reported

Nicolet-MX 1 Fourier Transform Infra Red spectrometer coupled to the three mirror White optical system; <30 min; nitrates and aldehydes were detected transformation products

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subs	tance			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Low	The source and purity of the test substance were not reported or verified by analytical means.
Domain 2: Test Desig	gn			
	Metric 3:	Study Controls	Medium	Some concurrent control group details were not included; however, the lack of data was not likely to have a substantial impact on study results.
			G 41 1	

		continu	ied from previou	s page
Study Citation:	Andersson, Y., L	jungstrom, E. (1967). Gas phase reaction of	f the NO3 radical	with organic compounds in the dark. Atmospheric Environment 23(5):1153-
OECD Harris and	1155.			
OECD Harmonized	Photolysis in Air			
Template:	5705075			
HERO ID:	5705275			
			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 3: Test Condition	ons			
Domain 5. Test Conditi	Metric 5:	Test Method Suitability	Medium	The test method was suitable for the test substance with minor deviations.
	Metric 6:	Testing Conditions	Medium	There were reported deviations or omissions in testing conditions.
	Metric 7:	Testing Consistency	High	Test conditions were consistent across samples or study groups.
	Metric 8:	System Type and Design	Medium	The system type and design were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 4: Test Organis	ms			
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
		2 mark - 1108 mark		
Domain 5: Outcome As	sessment			
	Metric 11:	Test Substance Identity	Medium	Nitrate radical reaction rates were reported in dark conditions; the photodegradation half-lives were not reported.
	Metric 12:	Test Substance Purity	Medium	The sampling methods were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 6: Confounding	2/Variable Control			
	Metric 13:	Confounding Variables	Low	Sources of variability and uncertainty in the measurements and statistical techniques and between study groups were not considered or accounted for in data evaluation resulting in some uncertainty.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Present	ation and Analysis			
	Metric 15:	Data Reporting	High	The target chemical concentrations were reported.
	Metric 16:	Statistical Methods and	Medium	Details regarding statistical methods and kinetic calculations were not fully reported, bu
		Kinetic Calculations		the omissions were not likely to have a substantial impact on study results.
Domain 8: Other				
Domain o. Oute	Metric 17:	Verification or Plausibility of Results	Medium	The study results were reasonable; however no blanks or reference compounds were included in this experiment.
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.
		-	ued on next page	

Study Citation: Andersson, Y., Ljungstrom, E. (1967). Gas phase reaction of the NO3 radical with organic compounds in the dark. Atmospheric Environment 23(5):1153-

1155

OECD Harmonized Photolysis in Air

Template:

HERO ID: 5705275

EVALUATION
Domain Metric Rating Comments

Overall Quality Determination Medium

Study Citation: Andersson, Y., Ljungström, E. (1989). Gas phase reaction of the NO3 radical with organic compounds in the dark. Atmospheric Environment (1967)

23(5):1153-1155. Photolysis in Air

Results Remarks, Sample time Results, Results not reported; not reported; not reported

OECD Harmonized Template:

HERO ID:

Deviation Results

Details

5675250

EXTRACTION

EXTRACTION			
Parameter	Data		
CASRN and Test Material	Not Reported; 1,3-butadiene		
Confidentiality, Type, Guideline	No; experimental; other: Non-guideline: gas-phase reaction with NO3 radical in the dark		
Solvent, Reactivity, Storage, Stability	NR; NR; NR		
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR		
Duration and Test Temperature	ca. 28 minutes; 296±1K		
Light Source, Intensity, and additional light de- tails	not reported; not reported		
Source Wavelength Lower and Upper	not reported; not reported		
Test Details and Control	Conducted in N2 atmosphere at standard pressure; N2O5 used as source for NO3 radicals; experimental set-up described previously; not reported		
Initial Concentration, Reference	ca. 1.7x10^15 molecule/cm3; not reported		
Compound			
Substance Wavelength Lower and Upper	not reported; not reported		
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	not reported; not reported		
Indirect Type Results, Indirect Rate	NO3 radical rate constant (cm3/molecule sec); rate constant k dependent on $k2/k-2$ (K2); $k = 5.6 \pm 0.8 \times 10^{-14}$ (K2 value at 296K from Malko and		
Constant Lower and Upper	Troe 1982); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 5.2 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$ (K2 value at 298K = 1.87x10^-11 cm3/molecule); $k = 4.4 \times 10^{-14}$		
	$= 7.9 \times 10^{-14}$ (K2 at 298K = 3.35×10 ⁻¹¹ cm3/molecule)		
Method Details Results and Products	IR spectra recorded using FTIR spectrometer; not reported		
Details Results Parameter Value and Parameter Results	test material concentrations; Approximate rate constant k4 was estimated from the slope of plotting ln([org]0/[org]t) vs (k-2[N2O5]t)/(k2[NO2]t)+k4[org]t)t; k4 was fit by least squares to observed N2O5 and org concentrations over time.		
Reference Substance Results, Percent Degradation Results and Standard	not reported; not reported; indicated error reported = two standard deviations		

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Test Substa	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	Low	The source and purity were not reported.
Domain 2: Test Design	1			
	Metric 3:	Study Controls	Low	Controls were not included.
			Continued on next	page

Study Citation: Andersson, Y., Ljungström, E. (1989). Gas phase reaction of the NO3 radical with organic compounds in the dark. Atmospheric Environment (1967)

OECD Harmonized

23(5):1153-1155. Photolysis in Air

Template: HERO ID: 567:

5675250

HERO ID:	5675250			
		I	EVALUATIO:	N
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported.
Domain 3: Test Cond	litions			
	Metric 5:	Test Method Suitability	High	The test method was suitable.
	Metric 6:	Testing Conditions	High	Testing conditions were reported.
	Metric 7:	Testing Consistency	N/A	This metric is not applicable to this study type.
	Metric 8:	System Type and Design	Medium	Some detail was omitted regarding the system set up; additional information may be found in cited work.
Domain 4: Test Organ	nisms			
C	Metric 9:	Outcome Assessment Methodology	N/A	This metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	This metric is not applicable to this study type.
D : 5 O :				
Domain 5: Outcome	Assessment Metric 11:	Test Substance Identity	Hiab	
	Metric 11:	Test Substance Identity Test Substance Purity	High N/A	The outcome assessment methodology addressed the intended outcome of interest. This metric is not applicable to this study type.
	Metric 12.	Test Substance I unity	IV/A	This metric is not applicable to this study type.
Domain 6: Confound	ing/Variable Control			
	Metric 13:	Confounding Variables	N/A	This metric is not applicable to this study type.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric is not applicable to this study type.
		Exposure		
Domain 7: Data Preso	entation and Analysis			
	Metric 15:	Data Reporting	Medium	Analytical details were not reported.
	Metric 16:	Statistical Methods and	High	Calculations were described.
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	High	Reported values were reasonable.
	Matria 10.	Results	N/A	This was this is not a multi-ship to this to the town
	Metric 18:	QSAR Models	IN/A	This metric is not applicable to this study type.
Overall Qua	lity Determin	ation	High	

Study Citation: EC, (2002). Summary risk assessment report for 1,3-butadiene.

OECD Harmonized

Photolysis in Air

Template:

EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, Guideline	no; estimated; other: not reported			
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported			
Duration and Test Temperature	Not Reported; Not Reported			
Light Source, Intensity, and additional light de-	Not Reported; Not Reported			
tails Source Wavelength Lower and Upper	Not Reported; Not Reported			
Test Details and Control	Not Reported; Not Reported			
Initial Concentration, Reference	Not Reported Not Reported; Not Reported			
Compound				
Substance Wavelength Lower and Upper	Not Reported; Not Reported			
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported			
Indirect Type Results, Indirect Rate	Reaction with Ozone; half-life = 1.9 days; Not Reported; Not Reported			
Constant Lower and Upper				
Method Details Results and Products Details Results	Not Reported; Not Reported			
Parameter Value and Parameter Results	Not Reported; Not Reported			
Reference Substance Results, Percent Degrada-	Not Reported; Not Reported			
tion Results and Standard				
Deviation Results Results Remarks, Sample time Results, Results	Not Reported; Not Reported; Not Reported			
Details	Not Reported, Not Reported			

EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Test Substance				
Metric 1:	Test Substance Identity	High	The test substance was identified.	
Metric 2:	Test Substance Purity	Low	The test substance source was not reported; no citation for data.	
Domain 2: Test Design				
Metric 3:	Study Controls	Low	Details were not included; no citation reported.	
Metric 4:	Test Substance Stability	Low	Details were not included; no citation reported.	
Domain 3: Test Conditions				
Metric 5:	Test Method Suitability	Low	Details were not included; no citation reported.	
		Continued on next	page	

Study Citation: EC, (2002). Summary risk assessment report for 1,3-butadiene. **OECD Harmonized** Photolysis in Air **Template: HERO ID:** 7348613 **EVALUATION** Metric Domain Rating Comments Testing Conditions Metric 6: Low Details were not included; no citation reported. Metric 7: Testing Consistency N/A Estimated value from secondary source with no citation. Metric 8: System Type and Design N/A Estimated value from secondary source with no citation. Domain 4: Test Organisms Metric 9: N/A Outcome Assessment Methodology Not applicable to the study. Metric 10: Sampling Methods N/A Not applicable to the study. Domain 5: Outcome Assessment Metric 11: Test Substance Identity No methodology was reported; no citation. Low

N/A

Metric Metric		g Variables N/A omes Unrelated to N/A	Estimated value from secondary source with no citation. This metric does not apply to this study type.
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Test Substance Purity

Domain 7: Data	Presentation	and	Analysis

Domain 6: Confounding/Variable Control

Metric 12:

Metric 15:	Data Reporting	Low	Estimated value from secondary source with no citation.
Metric 16:	Statistical Methods and	Low	Estimated value from secondary source with no citation.
	Kinetic Calculations		

Domain 8: Other

Metric 17:	Verification or Plausibility of	Low	Due to limited information, evaluation of the reasonableness of the study results was not
	Results		possible.
Metric 18:	OSAR Models	NI/A	A OSAP model was not reported

The metric is not applicable to the study.

Overall Quality Determination

Low

^{*} Related References: no references citedData also found in Pubchem entry (cites NIST; NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). NIST Standard Reference and Gas Kinetics Databases, 2013 Release. Washington, DC: US Sec Commerce. Available, as of Mar 9, 2015)

Study Citation:

EC, (2002). Summary risk assessment report for 1,3-butadiene.

OECD Harmonized

Photolysis in Air

Template: HERO ID:

7348613

EXTR	ACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	no; estimated; other: not reported
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported
Duration and Test Temperature	Not Reported; Not Reported
Light Source, Intensity, and additional light de-	Not Reported; Not Reported
tails Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Not Reported; Not Reported
Initial Concentration, Reference Compound	Not Reported Not Reported; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Reaction with hydroxyl radicals; half-life = 5.8 hours; Not Reported; Not Reported
Method Details Results and Products Details Results	Not Reported; Not Reported
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degrada- tion Results and Standard Deviation Results	Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported

	EVALUATION					
Domain		Metric	Rating	Comments		
Domain 1: Test Substan	ce					
	Metric 1:	Test Substance Identity	High	The test substance was identified.		
	Metric 2:	Test Substance Purity	Low	The test substance source was not reported; no citation for data.		
Domain 2: Test Design						
	Metric 3:	Study Controls	Low	Details were not included; no citation reported.		
	Metric 4:	Test Substance Stability	Low	Details were not included; no citation reported.		
Domain 3: Test Condition	ons					
	Metric 5:	Test Method Suitability	Low	Details were not included; no citation reported.		
	Metric 6:	Testing Conditions	Low	Details were not included; no citation reported.		
	Metric 7:	Testing Consistency	N/A	Estimated value from secondary source with no citation.		
		C	ontinued on next	page		

Study Citation: EC, (2002). Summary risk assessment report for 1,3-butadiene. **OECD Harmonized** Photolysis in Air **Template: HERO ID:** 7348613 **EVALUATION** Metric Domain Rating Comments Metric 8: System Type and Design N/A Estimated value from secondary source with no citation. Domain 4: Test Organisms Metric 9: Outcome Assessment Methodology N/A Not applicable to the study. Metric 10: Sampling Methods N/A Not applicable to the study. Domain 5: Outcome Assessment Metric 11: Test Substance Identity No methodology was reported; no citation. Low Metric 12: Test Substance Purity N/A The metric is not applicable to the study.

N/A

N/A

Estimated value from secondary source with no citation.

Due to limited information, evaluation of the reasonableness of the study results was not

This metric does not apply to this study type.

A QSAR model was not reported.

Domain 7: Data Presentation and Analysis			
Metric 15:	Data Reporting	Low	Estimated value from secondary source with no citation.
Metric 16:	Statistical Methods and	Low	Estimated value from secondary source with no citation.
	Kinetic Calculations		

Overall Quality Determination

Domain 6: Confounding/Variable Control

Domain 8: Other

Metric 13:

Metric 14:

Metric 17:

Metric 18:

Confounding Variables

Exposure

Results

QSAR Models

Health Outcomes Unrelated to

Verification or Plausibility of

Low

Low

N/A

possible.

^{*} Related References: no references citedData also found in Pubchem entry (cites NIST; NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). NIST Standard Reference and Gas Kinetics Databases, 2013 Release. Washington, DC: US Sec Commerce. Available, as of Mar 9, 2015)

OECD Harmonized

Template:

HERO ID: 5155560

		EXTRACTION
Parameter	Data	

CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 25 C
Light Source, Intensity, and additional light de-	NR; NR; NR
tails	ND ND
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference	NR NR; NR
Compound	
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life	NR; Not Reported; NR
by Loss Lower and Upper	
Indirect Type Results, Indirect Rate	Second order rate constant for reaction with OH radicals; k=6.68E-11 cm^3/molecule*sec; NR
Constant Lower and Upper	
Method Details Results and Products	NR; NR
Details Results Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degrada- tion Results and Standard	NR; NR; NR
Deviation Results	
Results Remarks, Sample time Results, Results	NR; NR; NR
Details	

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substa	ance			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source
				cited.
Domain 2: Test Design	n			
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.

Continued on next page ...

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

Template:

Photolysis in Air

HERO ID:

5155560

	E	EVALUATION	
Domain	Metric	Rating	Comments
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms			
Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessment			
Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Variable Cont	rol		
Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
	Exposure		
Domain 7: Data Presentation and Analy	ysis		
Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
Metric 16:	Statistical Methods and	Medium	Statistical method was not reported; more details may be in the source cited.
	Kinetic Calculations		
Domain 8: Other			
Metric 17:	Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
Metric 18:	Results QSAR Models	N/A	A QSAR model was not reported.

^{*} Related References: Cites secondary source Atkinson1985 [HERO ID 38261]

OECD Harmonized

Template:

CAINACIUN	EXTRA	CTION
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Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Duration and Test Temperature	NR; NR
Light Source, Intensity, and additional light de-	NR; NR; NR
tails Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference	NR NR; NR
Compound	
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life	NR; Not Reported; NR
by Loss Lower and Upper	Consideration and constant for most form with a most form
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with ozone; k=6.1E-18 cm ³ /molecule*sec; NR
Method Details Results and Products	NR; NR
Details Results	
Parameter Value and Parameter Results	1.9 days; Half-life for reaction with atmospheric ozone
Reference Substance Results, Percent Degrada-	NR; NR; NR
tion Results and Standard	
Deviation Results Results Remarks, Sample time Results, Results	NR; NR; NR
Details	

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substar	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditi	ions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
			Continued on next page .	

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

Photolysis in Air

Template:
HERO ID: 5155560

			EVALUATION	
Domain		Metric	Rating	Comments
Metr	ric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
Metr	ric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
Metr	ric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
Metr	ric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
Metr	ric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessme		The color and the circ	M 11	
	ric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
Metr	ric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Varial	ble Control			
Metr	ric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
Metr	ric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Presentation a	nd Analysis			
Metr	ric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
Metr	ric 16:	Statistical Methods and	Medium	Statistical method was not reported; more details may be in the source cited.
		Kinetic Calculations		
Domain 8: Other				
Metr	ric 17:	Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
Metr	ric 18:	Results QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination

^{*} Related References: Cites secondary source Klopffer et al. 1988 [HERO ID 1939717]

OECD Harmonized

Template:

EXTRACTION			
Parameter	Data		
CASRN and Test Material	106-99-0; 1,3-butadiene		
Confidentiality, Type, Guideline	no; experimental; other: not specified		
Solvent, Reactivity, Storage, Stability	NR; NR; NR		
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR		
Duration and Test Temperature	NR; 295 K		
Light Source, Intensity, and additional light de-	NR; NR; NR		
tails	AID AID		
Source Wavelength Lower and Upper	NR; NR		
Test Details and Control	NR; NR		
Initial Concentration, Reference	NR NR; NR		
Compound			
Substance Wavelength Lower and Upper	NR; NR		
Direct Quantum Yield Results, Direct Half Life	NR; Not Reported; NR		
by Loss Lower and Upper			
Indirect Type Results, Indirect Rate	Second order rate constant for reaction with NO3 radicals; k=5.34E-13 cm^3/molecule*sec; NR		
Constant Lower and Upper			
Method Details Results and Products	NR; NR		
Details Results Parameter Value and Parameter Results	NR; NR		
Reference Substance Results, Percent Degrada-	NR; NR		
tion Results and Standard	IR, IR, IR		
Deviation Results			
Results Remarks, Sample time Results, Results	NR; NR; NR		
Details			

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substa	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Condit	ions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
			Continued on next page	

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

OECD Harmonized Photolysis in Air

Template: 5155560

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organis	ms			
· ·	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome As	sessment			
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding	/Variable Control			
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Present	ation and Analysis			
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and	Medium	Statistical method was not reported; more details may be in the source cited.
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	Results QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination

^{*} Related References: Cites secondary source Atkinson and Carter 1984 [HERO ID 38267]

OECD Harmonized

Photolysis in Air

Template:

	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 298 +/- 2 K
Light Source, Intensity, and additional light de-	NR; NR; NR
tails Source Wavelength Lower and Upper	NR; NR
Test Details and Control	Environmental chamber under simulated atmospheric conditions; NO present at 0.11-2.4 ppm; NR
Initial Concentration, Reference Compound	0.5, 1.0, 2.0 ppm; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate	NR; NR; NR
Constant Lower and Upper	
Method Details Results and Products	NR; NR
Details Results Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard	NR; NR; NR
Deviation Results Results Remarks, Sample time Results, Results Details	NR; NR; Acrolein and NO2 identified as primary stable photoproducts.

·		·	EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subst	ance			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Desig	*			
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Condi	itions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
		C	ontinued on next page	

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

OECD Harmonized Photolysis in Air

Template: 5155560

			EVALUATION	
Domain		Metric	Rating	Comments
Metr	ric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
Metr	ric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
Metr	ric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms				
Metr	ric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
Metr	ric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Assessme		The color and the circ	M 11	
	ric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
Metr	ric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/Varial	ble Control			
Metr	ric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
Metr	ric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Presentation a	nd Analysis			
Metr	ric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
Metr	ric 16:	Statistical Methods and	Medium	Statistical method was not reported; more details may be in the source cited.
		Kinetic Calculations		
Domain 8: Other				
Metr	ric 17:	Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
Metr	ric 18:	Results QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination

^{*} Related References: Cites secondary source Maldotti et al 1980 [HERO ID 5747014].

OECD Harmonized

Photolysis in Air

Template:

HERO ID: 5155560

	EXTRACTION
Data	

Results Remarks, Sample time Results, Results NR; NR; NR

Details

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 305 K
Light Source, Intensity, and additional light de-	NR; NR; NR
tails Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference	NR NR; NR
Compound	
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life	NR; NR
by Loss Lower and Upper	
Indirect Type Results, Indirect Rate	Second order rate constant for reaction with OH radicals; kOH=6.79E-11 cm^3/molecule*sec; NR
Constant Lower and Upper	
Method Details Results and Products	NR; relative to n-butane (k=2.69E-12 cm ³ / molecules* s
Details Results	AND AND
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degrada-	NR; NR
tion Results and Standard	
Deviation Results	ND ND ND

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subst	ance			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Desig	,			
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Cond	itions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
			Continued on next page	

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

OECD Harmonized Photolysis in Air

Template: 5155560

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Orga	nisms			
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome	Assessment			
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confound	ling/Variable Control			
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Pres	entation and Analysis			
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and	Medium	Statistical method was not reported; more details may be in the source cited.
		Kinetic Calculations		• • • • • • • • • • • • • • • • • • • •
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	Results QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination

^{*} Related References: Cites secondary source Lloyd et al., 1976 [HERO ID 8541109]

OECD Harmonized Template:

HERO ID: 5155560

		EXTRACTION
Parameter	Data	

NR; NR

NR; NR; NR

CASRN and Test Material 106-99-0; 1,3-butadiene

Confidentiality, Type, Guideline no; experimental; other: not specified

Solvent, Reactivity, Storage, Stability NR; NR; NR; NR

Radiolabel, Source, State, Purity NR; NR; NR; NR Notes: NR

Duration and Test Temperature NR; 299.5 K Light Source, Intensity, and additional light de-NR; NR; NR Source Wavelength Lower and Upper NR; NR

Test Details and Control NR; NR Initial Concentration, Reference NR NR; NR Compound

Substance Wavelength Lower and Upper

Direct Quantum Yield Results, Direct Half Life NR; NR; NR

by Loss Lower and Upper

Indirect Type Results, Indirect Rate Second order rate constant for reaction with OH radicals; kOH=6.85E-11 cm^3/molecule*sec; NR

Constant Lower and Upper

Method Details Results and Products NR; absolute rate method

Details Results

Parameter Value and Parameter Results NR; NR Reference Substance Results, Percent Degrada-NR; NR; NR tion Results and Standard

Deviation Results

Results Remarks, Sample time Results, Results

Details

		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1	Test Substance Identity	High	The test substance was identified definitively.
Metric 2	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design			
Metric 3	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited
Metric 4	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions			
Metric 5	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.

Study Citation: ECB, (2002). European Union risk assessment report: 1,3-butadiene. **OECD Harmonized** Photolysis in Air **Template: HERO ID:**

5155560

		1	EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organis	ms			
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome As	sessment			
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding	g/Variable Control			
•	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Present	ation and Analysis			
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Statistical method was not reported; more details may be in the source cited.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	Results QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination

^{*} Related References: Cites secondary source Atkinson R, Perry RA, Pitts JN Jr. (1977). J Chem Phys. 67; 3170 [Not in HERO at the time of extraction]

OECD Harmonized

Template:

EXTR	ACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Duration and Test Temperature	NR; ~300 K
Light Source, Intensity, and additional light de- tails	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with OH radicals; kOH=6.51E-11 cm ³ /molecule*sec; NR
Method Details Results and Products Details Results	NR; relative to ethene (k=8.45E-12 cm^3/molecule*sec
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degrada- tion Results and Standard Deviation Results	NR; NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

			EVALUATION		
Domain		Metric	Rating	Comments	
Domain 1: Test Substar	nce				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.	
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.	
Domain 2: Test Design					
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.	
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.	
Domain 3: Test Conditions					
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.	
Continued on next page					

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

OECD Harmonized Photolysis in Air

Template:

HERO ID: 5155560

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organ	isms			
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome A	Assessment			
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confoundi	ng/Variable Control			
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Prese	ntation and Analysis			
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and	Medium	Statistical method was not reported; more details may be in the source cited.
		Kinetic Calculations		· · · · · · · · · · · · · · · · · · ·
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	Results QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination

^{*} Related References: Cites secondary source Barnes I, Bastian V, Becker KH, Fink EH, Zabel F (1982). Reactivity studies of organic substances towardshydroxyl radicals under atmospheric conditions. Atmos Environ. 16; 545-550. [Not in HERO at the time of extraction] and Atkinson, 1985 [HERO ID 38261].

Template:

HERO ID: 5155560

EXTRACTION

EXTRACTION			
Parameter	Data		
CASRN and Test Material	106-99-0; 1,3-butadiene		
Confidentiality, Type, Guideline	no; experimental; other: not specified		
Solvent, Reactivity, Storage, Stability	NR; NR; NR		
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR		
Duration and Test Temperature	NR; 297 K		
Light Source, Intensity, and additional light de-	NR; NR; NR		
tails Source Wavelength Lower and Upper	NR; NR		
Test Details and Control	NR; NR		
Initial Concentration, Reference	NR NR; NR		
Compound			
Substance Wavelength Lower and Upper	NR; NR		
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR		
Indirect Type Results, Indirect Rate	Second order rate constant for reaction with OH radicals; kOH=6.16E-11 cm^3/molecule*sec; kOH=6.88E-11 cm^3/molecule*sec		
Constant Lower and Upper			
Method Details Results and Products	NR; relative to propene (k=2.65E-11 cm ³ /molecule*sec and 2-methyl-2-butene (k=8.72E-11 cm ³ /molecule*sec		
Details Results Parameter Value and Parameter Results	NR; NR		
Reference Substance Results, Percent Degrada-	NR; NR		
tion Results and Standard			
Deviation Results			
Results Remarks, Sample time Results, Results Details	NR; NR		
Details			

			EVALUATION		
Domain		Metric	Rating	Comments	
Domain 1: Test Substar	nce				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.	
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.	
Domain 2: Test Design					
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.	
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.	
Domain 3: Test Conditions					
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.	
Continued on next page					

Study Citation: ECB, (2002). European Union risk assessment report: 1,3-butadiene. **OECD Harmonized** Photolysis in Air **Template: HERO ID:** 5155560 **EVALUATION** Metric Domain Rating Comments Testing Conditions Metric 6: Medium Testing conditions not reported; more details may be in the source cited. Metric 7: Testing Consistency Medium Details on this metric were not reported; more details may be in the source cited Metric 8: System Type and Design Medium System type and design not reported; more details may be in the source cited. Domain 4: Test Organisms Metric 9: Outcome Assessment Methodology N/A This metric does not apply to this study type. Metric 10: Sampling Methods N/A This metric does not apply to this study type Domain 5: Outcome Assessment Metric 11: Test Substance Identity Medium The outcome was reasonable; more details may be in the source cited. Metric 12: Test Substance Purity Medium Sampling details not reported; more details may be in the source cited. Domain 6: Confounding/Variable Control

Domain 7: Data Presentation and Analysis			
Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
Metric 16:	Statistical Methods and	Medium	Statistical method was not reported; more details may be in the source cited.
	Kinetic Calculations		

Domain 8: Other

Metric 17: Verification or Plausibility of Medium Values seem appropriate; more details may be in the source cited. Results QSAR Models N/A

Medium

N/A

Confounding variables not reported; more details may be in the source cited.

This metric does not apply to this study type.

A QSAR model was not reported.

Overall Quality Determination

Metric 18:

Metric 13:

Metric 14:

Confounding Variables

Exposure

Health Outcomes Unrelated to

^{*} Related References: Cites secondary source Ohta T (1983). J Phys Chem. 87; 1209 [Not in HERO at the time of extraction] and Atkinson 1985 [HERO ID 38261]

OECD Harmonized

Template: HERO ID:

5155560

EXTI	RAC	ΓΙΟΝ

	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 295 K
Light Source, Intensity, and additional light de-	NR; NR; NR
tails	NR; NR
Source Wavelength Lower and Upper	
Test Details and Control	NR; NR
Initial Concentration, Reference	NR NR; NR
Compound	
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life	NR; NR
by Loss Lower and Upper	
Indirect Type Results, Indirect Rate	Second order rate constant for reaction with OH radicals; kOH=6.65E-11 cm ³ /molecule*sec; Not Reported
Constant Lower and Upper	
Method Details Results and Products	NR; relative to propene (k=2.68E-11 cm^3/molecule*sec
Details Results Parameter Value and Parameter Results	ND, ND
	NR; NR
Reference Substance Results, Percent Degrada-	NR; NR
tion Results and Standard	
Deviation Results	ND, ND, ND
Results Remarks, Sample time Results, Results Details	NR; NR
Details	

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substar	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditi	ions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
			Continued on next page	

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

OECD Harmonized Photolysis in Air

Template: 5155560

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organ	nisms			
· ·	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome A	Assessment			
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confoundi	ng/Variable Control			
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Prese	entation and Analysis			
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and	Medium	Statistical method was not reported; more details may be in the source cited.
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	Results QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination

^{*} Related References: Cites secondary source Atkinson and Aschmann 1984 [HERO ID 8521463]

Template:

HERO ID: 5155560

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Duration and Test Temperature	NR; 295 K
Light Source, Intensity, and additional light de- tails	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	Second order rate constant for reaction with OH radicals; kOH=6.1E-11 cm^3/molecule*sec; kOH=6.8E-11 cm^3/molecule*sec
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	NR; NR
Results Remarks, Sample time Results, Results Details	NR; NR; NR

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subst	ance			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Desig	,			
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Cond	itions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
			Continued on next page	

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

OECD Harmonized Photolysis in Air

Template:

HERO ID: 5155560

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organi	isms			
· ·	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome A	assessment			
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confoundin	ng/Variable Control			
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Preser	ntation and Analysis			
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and	Medium	Statistical method was not reported; more details may be in the source cited.
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	Results QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination

^{*} Related References: Cites secondary source Becker KH, Biehl HM, Bruckman P et al. (1984). Methods of the ecotoxicological evaluation of chemicals. Photochemical degradation in the gas phase. Volume 6: OH reaction rate constants and tropospheric lifetimes of selected environmental chemicals. Report 1980-1983. Kernforschungsanlage Jülich GmbH, November 1983. [Not in HERO at the time of extraction]

OECD Harmonized

Template:

EXTRACTION				
Parameter	Data			
CASRN and Test Material	100 00 0, 1.2 haz ilian			
	106-99-0; 1,3-butadiene			
Confidentiality, Type, Guideline	no; experimental; other: not specified			
Solvent, Reactivity, Storage, Stability	NR; NR; NR			
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR			
Duration and Test Temperature	NR; NR			
Light Source, Intensity, and additional light de-	NR; NR; NR			
tails	ND ND			
Source Wavelength Lower and Upper	NR; NR			
Test Details and Control	NR; NR			
Initial Concentration, Reference	NR NR; NR			
Compound				
Substance Wavelength Lower and Upper	NR; NR			
Direct Quantum Yield Results, Direct Half Life	NR; NR; NR			
by Loss Lower and Upper				
Indirect Type Results, Indirect Rate	Second order rate constant for reaction with OH radicals; kOH=6.85E-11 cm ³ /molecule*sec; Not Reported			
Constant Lower and Upper				
Method Details Results and Products	NR; NR			
Details Results Parameter Value and Parameter Results	NR; NR			
Reference Substance Results, Percent Degrada-	NR; NR			
tion Results and Standard	TH, TH, TH			
Deviation Results				
Results Remarks, Sample time Results, Results	NR; NR			
Details				

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substance				
Meta	ric 1:	Test Substance Identity	High	The test substance was identified definitively.
Meti	ric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Design			25.11	
Meti		Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
Metr	ric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Conditions				
Meta	ric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
			Continued on next page	

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

OECD Harmonized Template:

5155560

EVALUATION Domain Metric Comments Rating Metric 6: **Testing Conditions** Medium Testing conditions not reported; more details may be in the source cited. Metric 7: Testing Consistency Medium Details on this metric were not reported; more details may be in the source cited Metric 8: System Type and Design Medium System type and design not reported; more details may be in the source cited. Domain 4: Test Organisms Metric 9: Outcome Assessment Methodology N/A This metric does not apply to this study type. Metric 10: Sampling Methods N/A This metric does not apply to this study type Domain 5: Outcome Assessment Metric 11: Test Substance Identity Medium The outcome was reasonable; more details may be in the source cited. Metric 12: Test Substance Purity Medium Sampling details not reported; more details may be in the source cited. Domain 6: Confounding/Variable Control Metric 13: Confounding Variables Medium Confounding variables not reported; more details may be in the source cited. Metric 14: Health Outcomes Unrelated to N/A This metric does not apply to this study type. Exposure Domain 7: Data Presentation and Analysis Metric 15: **Data Reporting** Medium Analytical method was not reported; more details may be in the source cited Metric 16: Statistical Methods and Medium Statistical method was not reported; more details may be in the source cited. Kinetic Calculations Domain 8: Other

Overall Quality Determination

Metric 17:

Metric 18:

Verification or Plausibility of

Results

QSAR Models

HERO ID:

Medium

Medium

N/A

Values seem appropriate; more details may be in the source cited.

A QSAR model was not reported.

^{*} Related References: Cites secondary source Funcke W (1979). Studie zur Erkennung des Zusammenhangs zwischen der Struktur einer chemischen Substanz undderen Anfaelligkeit fuer den Photoabbau. Forschungsbericht 10702003, Umweltbundesamt, Berlin. Quoted in FrankR (1986). Zusammenstellung einer Liste von kOH-Reaktionsgeschwindigkeitskonstanten aus Originalveroeffentlichungen fuer einzelne chemikalien und Bewertung des Verhaltens dieser Stoffe in der Troposphaere,Batelle-Institut, Frankfurt A. M., 11-12[Not in HERO at the time of extraction]

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

OECD Harmonized

[armonized Photolysis in Air

Template:

Details

EXTRACTION			
Parameter	Data		
CASRN and Test Material	106-99-0; 1,3-butadiene		
Confidentiality, Type, Guideline	no; experimental; other: not specified		
Solvent, Reactivity, Storage, Stability	NR; NR; NR		
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR		
Duration and Test Temperature	NR; NR		
Light Source, Intensity, and additional light de-	NR; NR; NR		
tails Source Wavelength Lower and Upper	NR; NR		
Test Details and Control	NR; NR		
Initial Concentration, Reference	NR NR; NR		
Compound			
Substance Wavelength Lower and Upper	NR; NR		
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; NR; NR		
Indirect Type Results, Indirect Rate	Second order rate constant for reaction with ozone; k=8.1E-18 cm^3/molecule*sec; k=8.4E-18 cm^3/molecule*sec		
Constant Lower and Upper	ND ND		
Method Details Results and Products Details Results	NR; NR		
Parameter Value and Parameter Results	NR; NR		
Reference Substance Results, Percent Degrada- tion Results and Standard	NR; NR; NR		
Deviation Results			
Results Remarks, Sample time Results, Results	NR; NR; NR		

·			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substa	ance			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	Test substance source and purity were not reported; more details may be in the source cited.
Domain 2: Test Desig				
	Metric 3:	Study Controls	Medium	No concurrent control group details reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported; more details may be in the source cited.
Domain 3: Test Condi	itions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
		C	Continued on next page	

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

OECD Harmonized Photolysis in Air

Template: 5155560

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details on this metric were not reported; more details may be in the source cited
· 	Metric 8:	System Type and Design	Medium	System type and design not reported; more details may be in the source cited.
Domain 4: Test Organisms	8			
-	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type
Domain 5: Outcome Asses	ssment			
	Metric 11:	Test Substance Identity	Medium	The outcome was reasonable; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Sampling details not reported; more details may be in the source cited.
Domain 6: Confounding/\	Variable Control			
	Metric 13:	Confounding Variables	Medium	Confounding variables not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Presentati	on and Analysis			
	Metric 15:	Data Reporting	Medium	Analytical method was not reported; more details may be in the source cited
	Metric 16:	Statistical Methods and	Medium	Statistical method was not reported; more details may be in the source cited.
		Kinetic Calculations		· · · · · · · · · · · · · · · · · · ·
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
	Metric 18:	Results QSAR Models	N/A	A QSAR model was not reported.

Overall Quality Determination

Medium

^{*} Related References: Cites secondary source Atkinson and Carter (1984) [HERO ID 38267]

Study Citation: Ghosh, B., Bugarin, A., Connell, B. T., North, S. W. (2010). OH radical initiated oxidation of 1,3-butadiene: isomeric selective study of the dominant

addition channel. Journal of Physical Chemistry A 114(16):5299-5305.

OECD Harmonized

Photolysis in Air

Template:

	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	none; experimental; other: non-guideline: OH radical oxidation in the presence of O2 and NO via laser photolysis
Solvent, Reactivity, Storage, Stability	NA; NA; NA
Radiolabel, Source, State, Purity	NA; Isomeric selective study starting with photodissociation (at 248 nm) of 2-iodo-but-3-en-1-ol which results in the hydroxy alkyl radical, OH-butadiene, the major addition product; 1-hydroxy-2-iodo-3-butene: colorless oil; NR Notes: 1-hydroxy-2-iodo-3-butene was synthesized from 57% hydroiodic acid and butadiene monoxide in water
Duration and Test Temperature	not specified; 298 ± 3 K
Light Source, Intensity, and additional light details	XE10 excimer laser (GAM Laser); not specified; not specified
Source Wavelength Lower and Upper	282 nm; 287 nm
Test Details and Control	NO concentration: 3.2E14 to 1.9E15 molecules/cm3; O2 concentration 6.5E15 to 6.5E16 molecules/cm3; not specified
Initial Concentration, Reference Compound	NA Not Reported; not reported
Substance Wavelength Lower and Upper	not specified; not specified
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	not specified; not specified
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Rate constant for the addition of O2 to the hydroxy alkyl radical: 7.0E-13 cm3/sec; Rate constant for the addition of NO to the hydroxy peroxy radical: 1.5E-11 cm3/sec
Method Details Results and Products Details Results	Analysis of time dependent OH/OD signals using laser photolysis-laser induced fluorescence (LP-LIF) method; isotopic cycling experiments conducted; end product yields: 7% organic nitrate (predicted, not directly measured), 63±10% acrolein, 21±9% 4-hydroxy-2-butenal, 9% 3-butenal, 63±10% HCHO
Parameter Value and Parameter Results	not reported; not reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	not reported; not reported
Results Remarks, Sample time Results, Results Details	Quantification of the branching between the E- and Z-isomers: the upper limit for E-isomer branching of the δ -hydroxy alkoxy radical was found to be $13\pm5\%$; not reported; not reported

EVALUATION					
Domain		Metric	Rating	Comments	
Domain 1: Test Subs	stance				
	Metric 1:	Test Substance Identity	High	The test substance was identified.	
	Metric 2:	Test Substance Purity	High	The source the test substance was reported.	
Domain 2: Test Desig	gn				
	Metric 3:	Study Controls	N/A	The study did not require concurrent control groups.	
		(Continued on next j	page	

	. Journal of Physical Chemistry A 114(16)		Comments The test substance preparation conditions were reported. The test method was suitable for the test substance. Testing conditions were reported. Test conditions were consistent.
44: 2.4: 2.5: 2.6: 2.7: 2.8:	Metric Test Substance Stability Test Method Suitability Testing Conditions Testing Consistency	Rating High High High High	Comments The test substance preparation conditions were reported. The test method was suitable for the test substance. Testing conditions were reported. Test conditions were consistent.
2 4: 2 5: 2 6: 2 7: 2 8:	Metric Test Substance Stability Test Method Suitability Testing Conditions Testing Consistency	Rating High High High High	Comments The test substance preparation conditions were reported. The test method was suitable for the test substance. Testing conditions were reported. Test conditions were consistent.
: 5: : 6: : 7: : 8:	Metric Test Substance Stability Test Method Suitability Testing Conditions Testing Consistency	Rating High High High High	Comments The test substance preparation conditions were reported. The test method was suitable for the test substance. Testing conditions were reported. Test conditions were consistent.
: 5: : 6: : 7: : 8:	Test Substance Stability Test Method Suitability Testing Conditions Testing Consistency	High High High High	The test substance preparation conditions were reported. The test method was suitable for the test substance. Testing conditions were reported. Test conditions were consistent.
: 5: : 6: : 7: : 8:	Test Method Suitability Testing Conditions Testing Consistency	High High High	The test method was suitable for the test substance. Testing conditions were reported. Test conditions were consistent.
2: 6: 2: 7: 2: 8:	Testing Conditions Testing Consistency	High High	Testing conditions were reported. Test conditions were consistent.
2: 6: 2: 7: 2: 8:	Testing Conditions Testing Consistency	High High	Testing conditions were reported. Test conditions were consistent.
: 7: : 8:	Testing Conditions Testing Consistency	High High	Test conditions were consistent.
8:	Testing Consistency	High	Test conditions were consistent.
	System Type and Design	_	The section time and decision course appropriate
: 9:		111g11	The system type and design were appropriate.
9:			
	Outcome Assessment Methodology	N/A	The metric is not applicable to the study.
: 10:	Sampling Methods	N/A	The metric is not applicable to the study.
	1 6		J
t			
: 11:	Test Substance Identity	Medium	There were minor differences between the assessment methodology and the intended outcome assessment.
: 12:	Test Substance Purity	High	The study reported the use of sampling methods that address the outcome of interest.
e Control			
: 13:	Confounding Variables	N/A	The metric is not applicable.
: 14:	Health Outcomes Unrelated to	N/A	The metric is not applicable.
	Exposure	1 1/11	The medie is not approache.
d Analysis			
: 15:	Data Reporting	High	Data reporting was appropriate.
: 16:	Statistical Methods and	Low	Statistical analysis and kinetic calculations were not described clearly.
	Kinetic Calculations		
: 17:	Verification or Plausibility of	High	The study results were reasonable.
	Results QSAR Models	N/A	A QSAR model was not reported.
: 18:	nation	High	
	e 17: e 18:	Kinetic Calculations 2 17: Verification or Plausibility of Results	Kinetic Calculations 2.17: Verification or Plausibility of High Results 2.18: QSAR Models N/A

verall	Quality Determination	His
yel all	Quality Determination	11

Study Citation: Greenwald, E. E., Park, J., Anderson, K. C., Kim, H., Reich, B. J., Miller, S. A., Zhang, R., North, S. W. (2005). The OH-initiated oxidation of 1,3-butadiene

in the presence of O2 and NO: a photolytic route to study isomeric selective reactivity. DUPE - Journal of Physical Chemistry A 109(35):7915-7922.

OECD Harmonized

Photolysis in Air

Template:

	EXTRACTION
Parameter	Data
CASRN and Test Material	Not Reported; 3-Buten-2-ol, 1-radical ion
Confidentiality, Type, Guideline	No; calculations; other: Non-guideline: RRKM/ME calculations correlated with experimental data
Solvent, Reactivity, Storage, Stability	NA; NA; NA
Radiolabel, Source, State, Purity	deuteration of the -OH group; test material was generated via photolysis of 1% 1-iodo-3-butene-2-ol in He (1 atm) (both non-deuterated and monodeuterated); Gas; NR Notes: 3-Buten-2-ol, 1-radical ion is the theoretical minor addition product of OH radical to 1,3-butadiene; to produce this radical ion as a major photolysis product, it was generated from photolysis of 1-iodo-3-butene-2-ol
Duration and Test Temperature	Pulsed; 298K (760 Torr)
Light Source, Intensity, and additional light de- tails Source Wavelength Lower and Upper	unfocused 266 nm beam from an Nd: YAG laser (Spectra Physics GCR-150-10); Not reported; The repetition rate of the lasers was set at 10 Hz and the delay between photolysis and probe lasers was controlled by a digital delay/ pulse generator 266 nm; Not reported
Test Details and Control	Laser photolysis/laser-induced fluorescence (LP/LIF) experiments used to produce activated adduct formed via OH addition to 1,3-butadiene; photodissociation dynamics via velocity-map imaging of 1-iodo-3-buten-2-ol were used for analysis via quantum chemical calculations using Gaussian 0341 software to provide all relevant energetics, geometries, and frequencies to obtain state counts as a function of energy for the OH-butadiene adduct radical cyclic isomerization reaction. Using RRKM theory coupled with master equation (ME) formalism reaction rate constants were calculated including branching ratios among isomers and further into the dissociative channel resulting in 1,3-butadiene and OH.; NA
Initial Concentration, Reference Compound	NA NA; Not reported
Substance Wavelength Lower and Upper	NA; NA
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not reported
Indirect Type Results, Indirect Rate Constant Lower and Upper Method Details Results and Products	distribution of hydroxyalkyl radicals: 70% beta, 30% alpha; radical rate constant for D-abstraction from alpha radical: CH2CHCH2CHOD + O2 -> CH2CHCH2CHO + DO2, k = 3.3x10^-11 molecules/cm3 sec; Not reported Not reported; Not Reported
Details Results	Not reported, Not Reported
Parameter Value and Parameter Results	Not reported; Not reported
Reference Substance Results, Percent Degrada- tion Results and Standard Deviation Results	Not reported; Not reported
Results Remarks, Sample time Results, Results Details	cyclic isomerization of beta-hydroxyalkyl radical to alpha-hydroxyalkyl radical was evident; Not reported; Not reported

EVALUATION					
Domain		Metric	Rating	Comments	
Domain 1: Test Sub	stance				
	Metric 1:	Test Substance Identity	Medium	The test substance was identified; however, the test substance was not specifically 1,3-butadiene.	
	Metric 2:	Test Substance Purity	N/A	The test substance was generated photolytically as part of the experiment.	
			Continued on next n	000	

		···continu	ied from pre	vious puge			
Study Citation:	Greenwald, E. E., Park, J., Anderson, K. C., Kim, H., Reich, B. J., Miller, S. A., Zhang, R., North, S. W. (2005). The OH-initiated oxidation of 1,3-butadiene in the presence of O2 and NO: a photolytic route to study isomeric selective reactivity. DUPE - Journal of Physical Chemistry A 109(35):7915-7922. Photolysis in Air						
OECD Harmonized							
Template:							
HERO ID:	5696791						
EVALUATION							
Domain		Metric	Rating	Comments			
Domain 2: Test Design							
· ·	Metric 3:	Study Controls	N/A	The metric is not applicable to this type of study.			
	Metric 4:	Test Substance Stability	N/A	The metric is not applicable to this type of study.			
Domain 3: Test Conditio	ins						
Domain 3. Test conditio	Metric 5:	Test Method Suitability	Low	Non-standard method evaluating transformation product; UV photolysis of iodohydrins.			
	Metric 6:	Testing Conditions	High	Testing conditions were monitored, reported, and appropriate for the method.			
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to this type of study.			
	Metric 8:	System Type and Design	N/A	The metric is not applicable to this type of study.			
Domain 4: Test Organism	ne						
Domain 4. Test Organisi	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this type of study.			
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this type of study.			
	1/104110 101	Sumpring Freurous	1,111	The means is not approvate to any type of stady.			
Domain 5: Outcome Ass	essment						
	Metric 11:	Test Substance Identity	Low	The outcome assessment methodology did not specifically address the intended outcome of interest; however, OH rate constant for a transformation product was reported.			
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to this type of study.			
Damain & Confounding	Wariahla Cantral						
Domain 6: Confounding	Metric 13:	Confounding Variables	N/A	The metric is not applicable to this type of study.			
	Metric 14:	Health Outcomes Unrelated to	N/A	The metric is not applicable to this type of study. The metric is not applicable to this type of study.			
	Wettic 14.	Exposure	IVA	The metric is not applicable to this type of study.			
Domain 7: Data Presenta	ntion and Analysis						
Domain 7. Data Freschia	Metric 15:	Data Reporting	High	Data reporting was appropriate.			
	Metric 16:	Statistical Methods and	High	Methods for kinetic calculations were described.			
	wieure 10.	Kinetic Calculations	High	riculous for kinetic calculations were described.			
Domain 8: Other							
	Metric 17:	Verification or Plausibility of	Low	Reported values were reasonable; however, not specific to the target chemical.			
	Metric 18:	Results QSAR Models	High	Model calculations were described.			
0 110 11	D						
Overall Qualit	y Determina	ation	Low				

OECD Harmonized

:380-381. Photolysis in Air

Template: HERO ID: 11779754

	EATRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	No; calculation; None
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Duration and Test Temperature	NR; NR
Light Source, Intensity, and additional light de- tails	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference	NR NR; NR
Compound Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life	NR; NR
by Loss Lower and Upper	
Indirect Type Results, Indirect Rate	NR; NR; NR
Constant Lower and Upper	NID NID
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degrada-	NR; NR; NR
tion Results and Standard	
Deviation Results Results Remarks, Sample time Results, Results	Half-lives in air = 0.76-7.8 hours (0.03 days-0.32 days). Based on measured photooxidation rate constant in air.; NR; NR
Details	Than 11465 in an = 0.76 7.5 hours (0.65 days-0.52 days). Dased on measured photocolidation rate constant in an., 146, 146

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subs	stance			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	The source and purity of the test substance were not reported; however, the omissions were not likely to have a substantial impact on the study results.
Domain 2: Test Design	gn			
	Metric 3:	Study Controls	Medium	Study controls were not reported and may affect the study results; however, the data are from a trusted secondary source.

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized :380-381. Photolysis in Air

Template: HERO ID:

11770754

HERO ID:	11779754			
		E	VALUATION	
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 3: Test Condi	itions			
	Metric 5:	Test Method Suitability	Medium	The test method was not reported; however, the data is from a trusted secondary source with reference to the source the calculation was based on.
	Metric 6:	Testing Conditions	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 7:	Testing Consistency	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 8:	System Type and Design	Medium	Equilibrium was not reported; however, the data are from a trusted secondary source.
Domain 4: Test Organ	nisms			
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome A	∆ ssessment			
Domain 3. Outcome 1	Metric 11:	Test Substance Identity	High	The outcome of interest was reported.
	Metric 12:	Test Substance Purity	Medium	The sampling method was not reported; however, the data are from a trusted secondary source.
Domain 6: Confoundi	ing/Variable Central			
Domain o. Comoundi	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty in the measurements were not reported; however, the omissions were not likely to have a substantial impact on study results.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Prese	entation and Analysis			
Domain 7. Data Hesc	Metric 15:	Data Reporting	Medium	Data reporting was limited, the analytical method was not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Kinetic and calculation details were not reported; however, the information is presented in a trusted secondary source.
Domain 8: Other				
Domain o. Other	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was no possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

:380-381. Photolysis in Air

Template: HERO ID:

OECD Harmonized

11779754

		EVALUATION		
Domain	Metric	Rating	Comments	
Overall Quality Determination		Medium		

^{*} Related References: Atkinson, R 1985; Atkinson, R and Carter, WPL 1984; Atkinson, R et al 1984A

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

:380-381. Photolysis in Air

Template:

OECD Harmonized

HERO ID: 11779754

HERO ID: 11/19/34	
	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	No; calculation; None
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Duration and Test Temperature	NR; NR
Light Source, Intensity, and additional light details	NR; NR; NR
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference	NR NR; NR
Compound	
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; Indirect half-life = 0.76 hours (0.03 days); Indirect half-life = 7.8 hours (0.32 days)
Indirect Type Results, Indirect Rate Constant Lower and Upper	NR; NR; NR
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	NR; NR
Reference Substance Results, Percent Degradation Results and Standard	NR; NR; NR
Deviation Results Results Remarks, Sample time Results, Results Details	Based on measured photooxidation rate constant in air with hydroxyl radicals, ozone, and nitrate radicals.; NR; NR

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subs	tance			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	The source and purity of the test substance were not reported; however, the omissions were not likely to have a substantial impact on the study results.
Domain 2: Test Desig	gn			
	Metric 3:	Study Controls	Medium	Study controls were not reported and may affect the study results; however, the data are from a trusted secondary source.
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.

Continued on next page ...

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized :380-381. Photolysis

:380-381. Photolysis in Air

Template:

]	EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Cond	itions			
	Metric 5:	Test Method Suitability	Medium	The test method was not reported; however, the data is from a trusted secondary source with reference to the source the calculation was based on.
	Metric 6:	Testing Conditions	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 7:	Testing Consistency	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 8:	System Type and Design	Medium	Equilibrium was not reported; however, the data are from a trusted secondary source.
Domain 4: Test Organ	nisms			
	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome	Assessment			
	Metric 11:	Test Substance Identity	High	The outcome of interest was reported.
	Metric 12:	Test Substance Purity	Medium	The sampling method was not reported; however, the data are from a trusted secondary source.
Domain 6: Confound	ing/Variable Control			
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty in the measurements were not reported; however, the omissions were not likely to have a substantial impact on study results.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Prese	entation and Analysis	·		
Domain 7. Data Trest	Metric 15:	Data Reporting	Medium	Data reporting was limited, the analytical method was not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Kinetic and calculation details were not reported; however, the information is presented in a trusted secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.
Overall Qua	lity Determin	nation	Medium	

^{*} Related References: Atkinson, R 1985; Atkinson, R and Carter, WPL 1984; Atkinson, R et al 1984A

Study Citation: Jenkin, M. E., Boyd, A. A., Lesclaux, R. (1998). Peroxy radical kinetics resulting from the OH-Initiated oxidation of 1,3-butadiene, 2,3-dimethyl-1,3-

butadiene and isoprene. Journal of Atmospheric Chemistry 29(3):267-298.

OECD Harmonized

Photolysis in Air

Template:

Details

	EXTRACTION
Parameter	Data
CASRN and Test Material	Not Reported; 1,3-butadiene
Confidentiality, Type, Guideline	No; experimental; other: Non-guideline: laser flash photolysis/UV absorption spectrometry for peroxy radical permutation reactions from OH-initiated oxidation of 1,3-butadiene
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; Aldrich; NR; >99% Notes: NR
Duration and Test Temperature	Not Reported; 298K (760 Torr)
Light Source, Intensity, and additional light de-	OH radicals were generated by the KrF excimer laser photolysis of H2O2; Not Reported; Not Reported
tails	040 N.D. (1
Source Wavelength Lower and Upper	248 nm; Not Reported
Test Details and Control	Not Reported; no absorption signals were detected at 270 nm in the absence of H2O2, indicating no absorbing species were formed from direct diene photolysis
Initial Concentration, Reference	9.0-26 10E16 molecule/cm3; Ethene
Compound	
Substance Wavelength Lower and Upper	Absorption-time profiles from the photolysis of the H2O2/diene/O2 mixtures recorded at 270-280 nm; Not Reported
Direct Quantum Yield Results, Direct Half Life	Not Reported; Not Reported
by Loss Lower and Upper	
Indirect Type Results, Indirect Rate	OH + 1,3-butadiene (+O2); OH + diene rate coefficients taken from reviews of Atkinson (1989; 1994); 6.66E-11 x 0.134 Rate coefficient x
Constant Lower and Upper	branching ratio (cm3/molecule sec); 6.66E-11 x 0.866 x 0.75 Rate coefficient x branching ratio (cm3/molecule sec)
Method Details Results and Products	Quantitative absorption-time profiles were simulated using the FACSIMILE program and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions and modeling of peroxy radicals via their permutation reactions are perfectly as a period of the
Details Results	tions and reactions with HO2 (and CH3O2, where appropriate).; Not Reported
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degrada-	Test system was run with ethene, results verified tje laser photolysis apparatuswas correctly aligned and functioning well; Not Reported; Not
tion Results and Standard	Reported
Deviation Results Results Remarks, Sample time Results, Results	Not Reported; Not Reported; Not Reported
results remains, sumple time results, results	1.00 Teepotees, 1.00 Teepotees

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subs	stance			
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	High	The source and purity of the test substance were reported.
Domain 2: Test Desi	ign			
	Metric 3:	Study Controls	Medium	Qualitative control results were reported.
			Continued on next page	

Study Citation:	Jenkin, M. E., Boyd, A. A., Lesclaux, R. (1998). Peroxy radical kinetics resulting from the OH-Initiated oxidation of 1,3-butadiene, 2,3-dimethyl-1,3-
	butadiene and isoprene. Journal of Atmospheric Chemistry 29(3):267-298.

OECD Harmonized Template:

Photolysis in Air

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 3: Test Cond	itions			
	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
	Metric 6:	Testing Conditions	High	Conditions were reported.
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to this study.
	Metric 8:	System Type and Design	High	The system was appropriate.
Domain 4: Test Organ	nisms			
_	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study.
Domain 5: Outcome	Assessment			
	Metric 11:	Test Substance Identity	Uninformative	Rate constant for intended outcome of interest is from another source and was not measured in this study.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to this study.
Domain 6: Confound	ing/Variable Control			
	Metric 13:	Confounding Variables	N/A	The metric is not applicable to this study.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study.
Domain 7: Data Prese	entation and Analysis			
	Metric 15:	Data Reporting	Low	Analytical details were omitted.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	The metric is not applicable to the study.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Uninformative	Results for outcome of interest are from a secondary source.
	Metric 18:	Results QSAR Models	N/A	The metric is not applicable to this study.
Overall Qua	lity Determin	ation	Uninformative	

Study Citation: Khaled, F., Giri, B. R., Liu, D., Assaf, E., Fittschen, C., Farooq, A. (2019). Insights into the Reactions of Hydroxyl Radical with Diolefins from Atmospheric

to Combustion Environments. Journal of Physical Chemistry A 123(11):2261-2271.

OECD Harmonized

Photolysis in Air

Template:

EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, Guideline	None; Experimental; other: Hydroxyl radical reactions			
Solvent, Reactivity, Storage, Stability	NR; NR; NR			
Radiolabel, Source, State, Purity	NR; NR; 99%			
Duration and Test Temperature	ca. 1.5 m-seconds; 294-438 K at 53 mbar (approximately); 881-1348 K at 1-2.5 bar approximately			
Light Source, Intensity, and additional light details	Excimer laser; measured but not reported; Lambda Physik LPX 201, operating at a repetition rate of 1 Hz and a laser fluence of ~70 mJ/cm2			
Source Wavelength Lower and Upper	248 nm for low temperature studies; 308 nm			
Test Details and Control	laser flash photolysis and laser-inducedfluorescence (LPFR/LIF) for lower temperature studies and shock tube and UV laser-absorption (ST/LA) for higher temperature studies that are not environmentally relevant; TBHP in argon (ST/LA technique); He/H2O2 mixture (LPFR/LIF technique)			
Initial Concentration, Reference Compound	15 ppm 70 ppm; Not reported			
Substance Wavelength Lower and Upper	Not reported; Not reported			
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not reported			
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not reported; Not reported			
Method Details Results and Products Details Results	Not reported; Not reported			
Parameter Value and Parameter Results	rate coefficients for the reaction of hydroxyl radicals; 7.96-4.86E-11 cm3/molecule second at 294-438 K			
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not reported; Not reported			
Results Remarks, Sample time Results, Results Details	Not reported; Not reported			

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Test Substar	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified by chemical name.
	Metric 2:	Test Substance Purity	High	The test substance source and purity were reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	High	A control experiment was reported.
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation, and storage conditions were not reported.

		contin	ued from pre	vious page	
Study Citation:	Khaled, F., Giri, B. R., Liu, D., Assaf, E., Fittschen, C., Farooq, A. (2019). Insights into the Reactions of Hydroxyl Radical with Diolefins from Atmospheric to Combustion Environments. Journal of Physical Chemistry A 123(11):2261-2271.				
OECD Harmonized	Photolysis in Air				
Template:					
HERO ID:	5618698				
]	EVALUATIO	N	
Domain		Metric	Rating	Comments	
Domain 3: Test Conditi	ons				
Domain 5. Test Conditi	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.	
	Metric 6:	Testing Conditions	Medium	Some details were omitted regarding testing conditions; however, this was not likely to	
	wienie o.	resumg conditions	Wicdiaiii	have influenced the interpretation of the results.	
	Metric 7:	Testing Consistency	High	This metric met the criteria for high confidence as expected for this type of study.	
	Metric 8:	System Type and Design	High	This metric met the criteria for high confidence as expected for this type of study.	
Domain 4: Test Organis	eme				
Domain 4. Test Organis	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.	
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type. The metric is not applicable to this study type.	
	Wictire 10.	Sampling Methods	IVA	The metric is not applicable to this study type.	
Domain 5: Outcome As	ssessment				
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed the outcomes of interest.	
	Metric 12:	Test Substance Purity	Medium	Details regarding sampling methods were not fully reported; however, the omissions were not likely to have a substantial impact on results.	
Domain 6: Confounding	g/Variable Central				
Domain o. Comounting	Metric 13:	Confounding Variables	N/A	No confounding variables were noted.	
	Metric 14:	Health Outcomes Unrelated to	N/A	The metric is not applicable to this study type.	
	Micure 14.	Exposure Exposure	IV/A	The metric is not applicable to this study type.	
Domain 7: Data Present	tation and Analysis				
	Metric 15:	Data Reporting	Medium	Some experimental data and half-life data was not reported.	
	Metric 16:	Statistical Methods and	Medium	The kinetic calculations were not described in detail but are assumed to be adequate.	
		Kinetic Calculations		. 1	
Domain 8: Other					
Domain o. Omei	Metric 17:	Verification or Plausibility of	High	The study results were reasonable.	
	wictic 17.	Results	ingii	The study results were reasonable.	
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.	
Overall Quali	ty Determin	nation	High		
Over an Quan	iy Determin	1411011	mgn		

Study Citation:	Klamt, A. (1993).	Estimation of gas-phase hydroxyl radical rate constants of organic compounds from molecular orbital calculations.	Chemosphere
	26(7):1273-1289		

OECD Harmonized

Template:

HERO ID: 660158

Photolysis in Air

EXTR	ACTION

EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; Structural Estimation			
Confidentiality, Type, Guideline	None; QSAR; other: Estimation of gas-phase hydroxyl radical rate constants using molecular orbital calculations			
Solvent, Reactivity, Storage, Stability	NA; NA; NA			
Radiolabel, Source, State, Purity	NA; NA; NA Notes: Estimation based on functional groups in chemical			
Duration and Test Temperature	Not reported; Not reported			
Light Source, Intensity, and additional light details	Not reported; Not reported			
Source Wavelength Lower and Upper	Not reported; Not reported			
Test Details and Control	OH rate constants determined using quantitative relationships between MO-based descriptors for electronic properties of reaction sites and rate constants for OH-radical reaction mechanisms.; Not reported			
Initial Concentration, Reference	Not reported Not reported; Experimental data for comparison			
Compound				
Substance Wavelength Lower and Upper	Not reported; Not reported			
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not reported			
Indirect Type Results, Indirect Rate Constant Lower and Upper	Hydroxyl radical rate constant; 83.4; Not reported			

of 2000 20 mer und opper	
Indirect Type Results, Indirect Rate	Hydroxyl radical rate constant; 83.4; Not reported
Constant Lower and Upper	
Method Details Results and Products	Rate constant for OH radical addition to olefinic carbon-carbon double bonds (sp2-carbon atoms); Not reported
Details Results	
Parameter Value and Parameter Results	Not reported; Rate constant units: 10E-12 cm3/molecule/s
Reference Substance Results, Percent Degrada-	66.9; Not reported; s = 0.28; r-squared = 0.954
tion Results and Standard	

Test Substance Stability

Deviation Results Results Remarks, Sample time Results, Results Not reported; Not reported

Metric 4:

Details

Domain Domain 1: Test Substance

Domain 2: Test Design

		EVALUATIO	N	
	Metric	Rating	Comments	
ce				
Metric 1:	Test Substance Identity	High	The test substance was definitively identified.	
Metric 2:	Test Substance Purity	N/A	The metric is not applicable to this study type.	
Metric 3:	Study Controls	N/A	The metric is not applicable to this study type.	

The metric is not applicable to this study type.

Continued on next page ...

N/A

Study Citation: Klamt, A. (1993). Estimation of gas-phase hydroxyl radical rate constants of organic compounds from molecular orbital calculations. Chemosphere 26(7):1273-1289. Photolysis in Air

OECD Harmonized	Photolysis in Air			
Template:				
HERO ID:	660158			
			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 3: Test Condition	ons		-	
	Metric 5:	Test Method Suitability	N/A	The metric is not applicable to this study type.
	Metric 6:	Testing Conditions	N/A	The metric is not applicable to this study type.
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to this study type.
	Metric 8:	System Type and Design	High	This metric met the criteria for high confidence as expected for this type of study.
D : 4 T : 0 :				
Domain 4: Test Organis	ms Metric 9:	Outcome Assessment Methodology	NT/A	The models is not conficult, to this study time
	Metric 9: Metric 10:	Outcome Assessment Methodology Sampling Methods	N/A N/A	The metric is not applicable to this study type. The metric is not applicable to this study type.
	Metric 10.	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Ass	sessment			
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed or reported the intended outcome of interest.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to this study type.
Domain 6: Confounding			27/1	
	Metric 13:	Confounding Variables	N/A	The metric is not applicable to this study type.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Present	ation and Analysis			
	Metric 15:	Data Reporting	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Statistical analysis reported and acceptable.
Domain 8: Other				
Bomain of Guier	Metric 17:	Verification or Plausibility of	High	The study results were reasonable.
	Metric 18:	Results QSAR Models	High	The QSAR model had a defined, unambiguous endpoint and parameters of model performance were reported.
Overall Qualit	Overall Quality Determination High			

Study Citation: Liu, X., Jeffries, H. E., Sexton, K. G. (1999). Hydroxyl radical and ozone initiated photochemical reactions of 1,3-butadiene. Atmospheric Environment

33(18):3005-3022.

OECD Harmonized Template:

Photolysis in Air

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Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	None; Experimental; other: Mechanistic study of the reactions of 1,3-butadiene with hydroxy radicals and ozone in the presence of nitrogen oxides
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR; 99%
Duration and Test Temperature	ca. 10 hours; 25°C (indoor experiment)
Light Source, Intensity, and additional light details	Natural light; day Sept 19, 1997, night Oct 7, 1997; UVA340, F40BL black and Vitalite full spectrum lamps (indoor experiment); Not reported; Not reported
Source Wavelength Lower and Upper	Not reported; Not reported
Test Details and Control	Ozone was injected during the experiment at a constant rate of 0.33 ppm/h.; Not reported
Initial Concentration, Reference Compound	10 ppm Not reported; Not reported
Substance Wavelength Lower and Upper	Not reported; Not reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not reported; Not reported
Method Details Results and Products Details Results	Analytical derivative method (O-(2,3,4,5,6-pentfluorobenzyl)-hydroxylamine (PFBHA) coupled with gas chromatography (GC)/ion trap mass spectrometry (MS) separation and detection; Transformation products: 1,3-butadiene monoxide, 1,3-butadiene diepoxide, furan, glycolaldehyde, glycidaldehyde, glycoxal, malonaldehyde, butendial, C4 unsaturated hydroxy carbonyl, hydroxy acetone, glycidaldehyde, 3-hydroxy-propanaldehyde, formaldehyde, acetaldehyde, acrolein, methylglyoxal, 2,3-butadione
Parameter Value and Parameter Results	Not reported; Not reported
Reference Substance Results, Percent Degradation Results and Standard Deviation Results Results Remarks, Sample time Results, Results	Not reported; Not reported; Not reported Not reported; Not reported; Indoor experiments of OH-initiated photodegradation resulted in the same outcome.
Details	

EVALUATION					
Domain		Metric	Rating	Comments	
Domain 1: Test Substance	ce				
	Metric 1:	Test Substance Identity	High	The test substance was definitively identified.	
	Metric 2:	Test Substance Purity	High	The test substance purity was reported. The test substance source was not reported.	
Domain 2: Test Design					
	Metric 3:	Study Controls	Medium	Some concurrent control group details were not included; however, the lack of data was not likely to have a substantial impact on study results.	

Study Citation: Liu, X., Jeffries, H. E., Sexton, K. G. (1999). Hydroxyl radical and ozone initiated photochemical reactions of 1,3-butadiene. Atmospheric Environment 33(18):3005-3022.

OECD Harmonized

Photolysis in Air

Template: HERO ID:

HERO ID:	598253			
]	EVALUATIO	N
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 3: Test Con	ditions			
	Metric 5:	Test Method Suitability	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 6:	Testing Conditions	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 7:	Testing Consistency	High	This metric met the criteria for high confidence as expected for this type of study.
	Metric 8:	System Type and Design	High	This metric met the criteria for high confidence as expected for this type of study.
Domain 4: Test Orga	anisms			
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome	e Assessment			
	Metric 11:	Test Substance Identity	Low	Quantitative data not reported for photodegradation rates or formation of transformation
	Metric 12:	Test Substance Purity	High	products. This metric met the criteria for high confidence as expected for this type of study.
	Wietite 12.	Test Substance Furity	Ingn	This metric met the effects for high confidence as expected for this type of study.
Domain 6: Confound	ding/Variable Control			
	Metric 13:	Confounding Variables	N/A	No confounding variables were noted.
	Metric 14:	Health Outcomes Unrelated to	N/A	The metric is not applicable to this study type.
		Exposure		
Domain 7: Data Pres	sentation and Analysis			
	Metric 15:	Data Reporting	Low	Degradation of test substance shown; however, quantitative data not reported for photodegradation rates or formation of transformation products.
	Metric 16:	Statistical Methods and Kinetic Calculations	Low	Data presented in figures as concentration over a time series.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	High	The transformation products identified were reasonable.
	Metric 18:	Results QSAR Models	N/A	The metric is not applicable to this study type.
Overall Qua	ality Determin	nation	Low	

Study	Citation:	Orlando, J. J., Tyndall, G. S., Apel, E. C., Riemer, D. D., Paulson, S. E. (2003), Rate coefficients and mechanisms of the reaction of Cl-atoms with a series

of unsaturated hydrocarbons under atmospheric conditions. International Journal of Chemical Kinetics 35(8):334-353.

OECD Harmonized Template:

Photolysis in Air

EXTRACTION				
Parameter	Data			
CASRN and Test Material	Not Reported; 1,3-butadiene			
Confidentiality, Type, Guideline	No; experimental; other: Non-guideline: photolysis of mixtures and reaction of Cl2 with 1,3-butadiene			
Solvent, Reactivity, Storage, Stability	NR; NR; NR			
Radiolabel, Source, State, Purity	NR; Aldrich; NR; ≥99% Notes: NR			
Duration and Test Temperature	Not reported; 296K (700 Torr)			
Light Source, Intensity, and additional light de- tails	Xe-arc lamp; Not reported; Not reported			
Source Wavelength Lower and Upper	235 nm; 400 nm			
Test Details and Control	Cl2 = 1.1–3.1E15 molecule/cm3; reaction vessel: stainless steel environmental chambers; Not reported			
Initial Concentration, Reference	ca. 2.8E15 molecule/cm3; Not reported			
Compound				
Substance Wavelength Lower and Upper	Not reported; Not reported			
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not reported			
Indirect Type Results, Indirect Rate	Not reported; Not reported			
Constant Lower and Upper				
Method Details Results and Products	FTIR and GC/MS; observed products: CH2O 7±1%, HCOCl 3±1%, and acrolein ca. 3%; other lab sorptions were observed but not specifically			
Details Results	identified, likely end products: chlorinated methyl vinyl ketone, HC(O)Cl, acrolein, 2-chloro-3-butenal, 4-chlorocrotonaldehyde, CH2O, CO, and CO2			
Parameter Value and Parameter Results	Not reported; Not reported			
Reference Substance Results, Percent Degrada-	Not reported; Not reported			
tion Results and Standard				
Deviation Results				
Results Remarks, Sample time Results, Results Details	Not reported; Not reported; Study results for 1,3-butadiene were not quantitative			

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subs	tance			
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	High	The source and purity of the test substance were reported.
Domain 2: Test Desi	gn			
	Metric 3:	Study Controls	Low	No controls were reported.
			Continued on next page	

		continu	ied from previous	page		
Study Citation:	Orlando, J. J., Tyndall, G. S., Apel, E. C., Riemer, D. D., Paulson, S. E. (2003). Rate coefficients and mechanisms of the reaction of Cl-atoms with a series of unsaturated hydrocarbons under atmospheric conditions. International Journal of Chemical Kinetics 35(8):334-353.					
OECD Harmonized	Photolysis in Air					
Template: HERO ID:	3254900					
HERO ID:	3234900					
ъ.			EVALUATION			
Domain	3.5	Metric	Rating	Comments		
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.		
Domain 3: Test Conditio	ons					
	Metric 5:	Test Method Suitability	High	The test method was suitable.		
	Metric 6:	Testing Conditions	High	Test conditions were reported.		
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to this study type.		
	Metric 8:	System Type and Design	High	The system was appropriate.		
Domain 4. Test Organism	~~					
Domain 4: Test Organism	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.		
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type. The metric is not applicable to this study type.		
Domain 5: Outcome Ass	sessment	1 0		7 VI		
	Metric 11:	Test Substance Identity	Low	Quantitative rate results were not reported.		
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to this study type.		
Domain 6: Confounding	/Variable Control					
Domain o. Comounting	Metric 13:	Confounding Variables	N/A	The metric is not applicable to this study type.		
	Metric 14:	Health Outcomes Unrelated to	N/A	The metric is not applicable to this study type.		
		Exposure	- "			
Domain 7: Data Presenta	ation and Analysis					
	Metric 15:	Data Reporting	Low	Limited detail regarding analytical method; percent recovery or mass balance were not reported.		
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	The metric is not applicable to this study.		
Domain 8: Other						
2 omain of other	Metric 17:	Verification or Plausibility of Results	Low	Quantitative rate results were not reported; however, transformation products were reported.		
	Metric 18:	QSAR Models	N/A	The metric is not applicable to this study type.		
Overall Qualit	y Determin	ation	Medium			

Study Citation:

Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

OECD Harmonized

Photolysis in Air

Template:

HERO ID: 5589165

	EXTRACTION				
Parameter	Data				
CASRN and Test Material	106-99-0; 1,3-butadiene				
Confidentiality, Type, Guideline	no; experimental; other: not specified				
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported				
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported				
Duration and Test Temperature	24 hr; 45-50°F				
Light Source, Intensity, and additional light de-	not specified; UV irradiation; Not Reported; Not Reported				
Source Wavelength Lower and Upper	Not Reported; Not Reported				
Test Details and Control	Air sample collected for irradiation: Ambient air, 12/22/65, 7:40-8:00 PST, light haze; Not Reported				
Initial Concentration, Reference Compound	9.0 ppb; Not Reported				
Substance Wavelength Lower and Upper	Not Reported; Not Reported				
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported				
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported				
Method Details Results and Products Details Results	Not Reported; Not Reported				
Parameter Value and Parameter Results	0 ppb; Concentration of butadiene after 24 hr UV Irradiation				
Reference Substance Results, Percent Degrada- tion Results and Standard Deviation Results	Not Reported; Not Reported				
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported				

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substa	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported.
Domain 2: Test Design	1			
	Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.

Domain 3: Test Conditions

Study Citation: OECD Harmonized Template:

Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

Photolysis in Air

HERO ID:

5589165

Overall Quality Determination

		F	EVALUATION	
Domain		Metric	Rating	Comments
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Orga	nisms			
C	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome	Assessment			
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology 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 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confound	ling/Variable Control			
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to	N/A	Rating of this factor is not applicable to this kind of information.
		Exposure		
Domain 7: Data Pres	entation and Analysis			
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

^{*} Related References: Cited from Stephens, Edgar R. and Frank R. Burleson, "Analysis of the Atmosphere for Light Hydrocarbons", J. APCA 17 (33), 147-53 (1967). [HERO ID 15208]

Medium

Study Citation: OECD Harmonized Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

Photolysis in Air

Template:

HERO ID: 5589165

EXTRACTION			
Parameter	Data		
CASRN and Test Material	106-99-0; 1,3-butadiene		
Confidentiality, Type, Guideline	no; experimental; other: not specified; photooxidation		
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported		
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported; Not Reported		
Duration and Test Temperature	not reported; 79°F		
Light Source, Intensity, and additional light de- tails	not reported; not reported; not reported		
Source Wavelength Lower and Upper	not reported; not reported		
Test Details and Control	In a long-path infrared spectrometer mixtures of N2, O2, NO, NO2, and butadiene were irradiated and formation of NO2 was monitored.; not reported		
Initial Concentration, Reference Compound	not reported; not reported		
Substance Wavelength Lower and Upper	not reported; not reported		
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	not reported; not reported		
Indirect Type Results, Indirect Rate Constant Lower and Upper	not reported; not reported		
Method Details Results and Products Details Results	not reported; not reported		
Parameter Value and Parameter Results	4.3 ppb/min; NO photooxidation rate in the presence of butadiene		
Reference Substance Results, Percent Degrada- tion Results and Standard Deviation Results	not reported; not reported		
Results Remarks, Sample time Results, Results Details	not reported; not reported; not reported		

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substar	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported; additional details may be in source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.

Domain 3: Test Conditions

Details

Continued on next page ...

Study Citation: OECD Harmonized Template: HERO ID: Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

Photolysis in Air

5589165

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Org	anisms			
C	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome				
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology 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 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confoun	ding/Variable Control			
Domain or Comoun	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to	N/A	Rating of this factor is not applicable to this kind of information.
		Exposure		
Domain 7: Data Pre	sentation and Analysis			
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and	Medium	No statistical methods or kinetic calculations were reported in the secondary source.
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

Medium

^{*} Related References: Cited from Glasson, William A. and Charles S. Tuesday, "Hydrocarbon Reactivities in the Atmospheric Photooxidation of Nitric Oxide",. Env. Sci.Technol. 4 (11), 916-24 (1970b). [HERO ID 14872]

Study Citation: OECD Harmonized Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

Photolysis in Air

Template:

CAINACIUN	EXTRA	CTION
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Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified; photooxidation
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported
Duration and Test Temperature	Not Reported; 29°C
Light Source, Intensity, and additional light de-	Not Reported; Not Reported; Not Reported
tails	N.D. (IN.D. (I
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Not Reported; Not Reported
Initial Concentration, Reference	Not Reported Not Reported; Not Reported
Compound Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life	Not Reported; Not Reported Not Reported; Not Reported
by Loss Lower and Upper	Not Reported, Not Reported
Indirect Type Results, Indirect Rate	Not Reported; Not Reported; Not Reported
Constant Lower and Upper	
Method Details Results and Products	Not Reported; Not Reported
Details Results Parameter Value and Parameter Results	0.44v100.2/mm min. Bata constant for NO thermal evidation
	0.44x10^-3/ppm min; Rate constant for NO thermal oxidation
Reference Substance Results, Percent Degrada- tion Results and Standard	Not Reported; Not Reported
Deviation Results	
Results Remarks, Sample time Results, Results	Acrolein and formaldehyde were identified as NO-butadiene reaction products.; Not Reported; Not Reported
Details	

		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified by name.
Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported in this secondary source.
Domain 2: Test Design	Study Control	M. Jane	
Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.
Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.

Study Citation: OECD Harmonized Template:

Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

Photolysis in Air

HERO ID:

5589165

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Orga	nisms			
<i>g.</i>	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome	Assassment			
Domain 5. Outcome	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology 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 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based of the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confound	ling/Variable Control			
Domain o. Comoune	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to	N/A	Rating of this factor is not applicable to this kind of information.
		Exposure		6
Domain 7: Data Pres	entation and Analysis			
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

Medium

^{*} Related References: Cited from Glasson, William A. and Charles S. Tuesday, "Atmospheric Thermal Oxidation of Nitric Oxide in the Presence of Dienes", Env. Sci. Technol. 4 (9), 752-57 (1970a).

Study Citation: OECD Harmonized Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

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Photolysis in Air

Template:

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported
Duration and Test Temperature	Not Reported; Not Reported
Light Source, Intensity, and additional light de-	Not Reported; Not Reported
tails Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Not Reported; Not Reported
Initial Concentration, Reference	Not Reported Not Reported; Not Reported
Compound	
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate	Not Reported; Not Reported; Not Reported
Constant Lower and Upper	
Method Details Results and Products	Rate of decrease of NO2 concentrations in the butadiene-air mixture was measured; Not Reported
Details Results Parameter Value and Parameter Results	0.4x10^-4/ppm min; Rate constant for NO2-butadiene reaction
Reference Substance Results, Percent Degradation Results and Standard Deviation Results	Not Reported; Not Reported
Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported

EVALUATION				
Domain		Metric	Rating	Comments
Domain 1: Test Substar	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.
Domain 3: Test Conditi	ions			
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.
			Continued on next page	•••

Study Citation: OECD Harmonized Template: Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

Photolysis in Air

HERO ID: 5589165

			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organ	nisms			
<i>8</i>	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
D : 5 0 :				
Domain 5: Outcome		Total Code and Identition	M - 4'	
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology 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 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confound	ing/Variable Control			
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Prese	entation and Analysis			
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

Overall Quality Determination

Medium

^{*} Related References: Cited from Glasson, William A. and Charles s. Tuesday, "Atmospheric Thermal Oxidation of Nitric Oxide in the Presence of Dienes", Env.Sci. Technol. 4 (9), 752-57 (1970a).

Study Citation: OECD Harmonized Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

Photolysis in Air

Template:

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported
Duration and Test Temperature	24 hr; 40-45°F
Light Source, Intensity, and additional light de-	Not Reported; Not Reported
Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Air sample collected for irradiation: Ambient air, 3/10/66, 8:05-8:25 PST, moderate haze; Control measured under same conditions in the dark. Starting concentration: 2.0 ppb; after 24 hr in dark: 2.0 ppb
Initial Concentration, Reference Compound	2.4 ppb; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported; Not Reported
Method Details Results and Products Details Results	Not Reported; Not Reported
Parameter Value and Parameter Results	0 ppb; Concentration of butadiene after 24 hr UV Irradiation
Reference Substance Results, Percent Degradation Results and Standard	Not Reported; Not Reported
Deviation Results Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Not Reported

	EVALUATION					
Domain		Metric	Rating	Comments		
Domain 1: Test Substa	nce					
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.		
	Metric 2:	Test Substance Purity	Medium	The test substance source and purity were not reported.		
Domain 2: Test Design	1					
	Metric 3:	Study Controls	Medium	Concurrent control group details were not reported in the secondary source.		
	Metric 4:	Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.		
Domain 3: Test Conditions						
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.		
	Continued on next page					

Study Citation: OECD Harmonized Template:

Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

Photolysis in Air

HERO ID:	3507105			
			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Orga	nisms			
	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome	Assessment			
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology is unknown but is likely to be appropriate base on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based of the data's inclusion in a peer-reviewed/recognized database or other secondary source
Domain 6: Confound	ing/Variable Control			
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Pres	entation and Analysis			
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognize database or other secondary source.
	Metric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Qua	lity Determin	ation	Medium	

^{*} Related References: Cited from Stephens, Edgar R. and Frank R. Burleson, "Analysis of the Atmosphere for Light Hydrocarbons", J. APCA 17 (33), 147-53(1967). [HERO ID 15208]

EXTRACTION

Study Citation:

Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

Not Reported; Not Reported; Not Reported

Not Reported; Not Reported; Not Reported

OECD Harmonized

Photolysis in Air

Template:

HERO ID: 5589165

Reference Substance Results, Percent Degrada-

Results Remarks, Sample time Results, Results

tion Results and Standard Deviation Results

Details

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	no; experimental; other: not specified
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported
Duration and Test Temperature	24 hr; 55-60°F
Light Source, Intensity, and additional light de-	not specified; UV irradiation; Not Reported; Not Reported
tails Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Air sample collected for irradiation: Ambient air, 3/10/66, 7:50-8:00 PST, heavy haze; Control measured under same conditions in the dark.
Initial Concentration, Reference	Starting concentration: 2.8 ppb; after 24 hr in dark; 2.6 ppb 2.6 ppb; Not Reported
Compound	
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life	Not Reported; Not Reported
by Loss Lower and Upper	
Indirect Type Results, Indirect Rate	Not Reported; Not Reported
Constant Lower and Upper Method Details Results and Products	Not Reported; Not Reported
Details Results	not reported, not reported
Parameter Value and Parameter Results	0 ppb; Concentration of butadiene after 24 hr UV Irradiation

EVALUATION					
Domain	Metric	Rating	Comments		
Domain 1: Test Substance					
Metric	1: Test Substance Identity	High	The test substance was identified by name.		
Metric 2	2: Test Substance Purity	Medium	The test substance source and purity were not reported.		
Domain 2: Test Design					
Metric 3	3: Study Controls	Medium	Concurrent control group details were not reported in the secondary source.		
Metric 4	4: Test Substance Stability	Medium	Test substance stability, homogeneity, preparation, and storage conditions were not reported in the secondary source.		
Domain 3: Test Conditions					
Metric :	5: Test Method Suitability	Medium	Test method details were not reported in the secondary source.		
		Continued on next page			

Study Citation: OECD Harmonized Template: HERO ID: Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.

Photolysis in Air

5589165

		E	CVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Testing conditions are unknown but are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 7:	Testing Consistency	Medium	Testing consistency is unknown but are likely to be appropriate based on the data's in clusion in a peer-reviewed/recognized database or other secondary source.
	Metric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organi	isms			
Domain 1. Test Organi	Metric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
		The first state of the first sta		
Domain 5: Outcome A	ssessment			
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology is unknown but is likely to be appropriate base on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based of the data's inclusion in a peer-reviewed/recognized database or other secondary source
Domain 6: Confoundir	ng/Variable Control			
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Preser	ntation and Analysis			
	Metric 15:	Data Reporting	Medium	Limited data is reported in the secondary source but study data are likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognize database or other secondary source.
		QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.

^{*} Related References: Cited from Stephens, Edgar R. and Frank R. Burleson, "Analysis of the Atmosphere for Light Hydrocarbons", J. APCA 17 (33), 147-53(1967). [HERO ID 15208]

Study Citation: Sexton, K. G., Doyle, M. L., Jeffries, H. E., Ebersviller, S. (2007). Development and testing of a chemical mechanism for atmospheric photochemical

transformations of 1,3-butadiene. Chemico-Biological Interactions 166(1-3):156-162.

OECD Harmonized

Photolysis in Air

Template:

HERO ID: 618974

112110 121				
EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, Type, Guideline	None; Experimental; other: Mechanistic study of the reactions of 1,3-butadiene with OH, NO3 and O3			
Solvent, Reactivity, Storage, Stability	NR; NR; NR			
Radiolabel, Source, State, Purity	NR; NR; NR			
Duration and Test Temperature	19 hours; 60-100, 38-79, 65-95°F			
Light Source, Intensity, and additional light de- tails	Natural sunlight; Not reported; 0.5, 0.7, 0.4 Langley's			
Source Wavelength Lower and Upper	Not applicable; Not applicable			
Test Details and Control	3 chamber experiments on 5/20/98, 5/20/2005, 9/17/97. % humidity: 46-55, 35-45, 54-57. Air samples from both hydroxyl- and ozone-initiated of photooxidized 1,2-butadiene were analyzed; Not reported			
Initial Concentration, Reference	1.513, 1.996, 1.120 ppm; Not applicable			
Compound				
Substance Wavelength Lower and Upper	Not applicable; Not applicable			
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not reported; Not applicable; Not applicable			
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not applicable; Not applicable			
Method Details Results and Products	Analyzed by derivatization with O-(2,3,4,5,6-pentafluorobenzyl)-hydroxylamine; GC-MS; Major products: acrolein, formaldehyde, furan, 1,3-			
Details Results	butadiene monoxide and an organic nitrate			
Parameter Value and Parameter Results	0.468, 0.495, 0.686; 0.258, 0.074, 0.097; ppm NO; NO2 formation			
Reference Substance Results, Percent Degrada- tion Results and Standard Deviation Results	Not applicable; Not applicable			
Results Remarks, Sample time Results, Results Details	Primary reactions of 1,3-butadiene with OH, NO3 and O3 were represented; 10, 6.8, 9 hours; Univ NC outdoor smog chamber			

EVALUATION				
Domain		Metric	Rating	Comments
Domain 1: Test Subst	tance			
	Metric 1:	Test Substance Identity	Medium	The test substance was identified by trade name or other internal designation, but characterization details were omitted that could affect interpretation of study results; however, the omission was not likely to have a substantial impact on the study results.
	Metric 2:	Test Substance Purity	Medium	The test substance source was not reported and the test substance purity was not reported; however, the omissions or identified impurities were not likely to have a substantial impact on the study results.

Domain 2: Test Design

Study Citation:	Sexton, K. G., Doyle, M. L., Jeffries, H. E., Ebersviller, S. (2007). Development and testing of a chemical mechanism for atmospheric photochemical
	transformations of 1,3-butadiene. Chemico-Biological Interactions 166(1-3):156-162.
OECD Harmonized	Photolysis in Air

OECD Harmonized
Template:
HERO ID:

HERO ID:	618974			
		I	EVALUATIO:	N
Domain		Metric	Rating	Comments
	Metric 3:	Study Controls	N/A	The metric is not applicable to this study type.
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.
Domain 3: Test Cond	litions			
	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
	Metric 6:	Testing Conditions	High	Testing conditions were monitored, reported, and appropriate for the method.
	Metric 7:	Testing Consistency	High	The conditions of the exposure were documented.
	Metric 8:	System Type and Design	High	The system type and design were capable of appropriately maintaining substance concentrations.
Domain 4: Test Orga	nisms			
	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
		1 0		11 771
Domain 5: Outcome	Assessment			
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed or reported the intended outcome of interest.
	Metric 12:	Test Substance Purity	High	The study reported the use of sampling methods that address the outcome(s) of interest, and used widely accepted methods/approaches for the chemical and media being analyzed and no notable uncertainties or limitations were expected to influence results.
Domain 6: Confound	ing/Variable Control			
Domain o. Comound	Metric 13:	Confounding Variables	N/A	No confounding variables were noted.
	Metric 14:	Health Outcomes Unrelated to	N/A	The metric is not applicable to this study type.
		Exposure		The means is not approvable to any study type.
Domain 7: Data Prese	entation and Analysis			
	Metric 15:	Data Reporting	Medium	The target chemical and transformation product(s) concentrations, extraction efficiency, percent recovery, or mass balance were not reported; however, these omissions were not likely to have a substantial impact on study results.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Statistical methods or kinetic calculations were clearly described and address the dataset.
Domain 8: Other				
Domain o. Onici	Metric 17:	Verification or Plausibility of	High	Reported values were within expected range as defined by reference substance.
	Metric 18:	Results QSAR Models	N/A	The metric is not applicable to this study type.

Study Citation: Sexton, K. G., Doyle, M. L., Jeffries, H. E., Ebersviller, S. (2007). Development and testing of a chemical mechanism for atmospheric photochemical

transformations of 1,3-butadiene. Chemico-Biological Interactions 166(1-3):156-162.

OECD Harmonized Template:

Photolysis in Air

		EVALUATION		
Domain	Metric	Rating	Comments	
Overall Quality De	termination	High		

Study Citation: Tuazon, E. C., Alvarado, A., Aschmann, S. M., Atkinson, R., Arey, J. (1999). Products of the gas-phase reactions of 1,3-butadiene with OH and NO3

radicals. Environmental Science & Technology 33(20):3586-3595.

OECD Harmonized

Photolysis in Air

Results Remarks, Sample time Results, Results Not Reported; 6.5 min; Not Reported

Template:

HERO ID: 1742345

	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	None; Experimental, OH radical, products reported, % loss degradation reported; None
Solvent, Reactivity, Storage, Stability	NA; NR; NR
Radiolabel, Source, State, Purity	NA; Aldrich Chemical Co.; NR; >/= 99.0%
Duration and Test Temperature	$2\text{-}7 \text{ min}; 298 \pm 2 \text{ K}$
Light Source, Intensity, and additional light details	Two parallel banks of black lamps; NR; 20% maximum light intensity used; NR
Source Wavelength Lower and Upper	300; NR
Test Details and Control	OH radicals generated by photolysis of methyl nitrite; NR
Initial Concentration, Reference	5.7 - 6.2E10^13 molecule/cm^3; NR
Compound	
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; NR; NR
Indirect Type Results, Indirect Rate Constant Lower and Upper	OH radical (in the presence of NO); NR; NR
Method Details Results and Products	7500 L Teflon chamber at ~5% relative humidity, samples analyzed by GC-FID; Acrolein (0.55 ± 0.05), HCHO (0.62 ± 0.05), Furan (0.03 -
Details Results	0.04), organic nitrates (0.07 $\hat{A}\pm$ 0.03)
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degrada- tion Results and Standard Deviation Results	Not Reported; 53%; NR

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substa	ance			
	Metric 1:	Test Substance Identity	High	The test substance was identified by name.
	Metric 2:	Test Substance Purity	High	The test substance source and purity were reported.
Domain 2: Test Desig	n			
	Metric 3:	Study Controls	Medium	Dark controls were not explicitly included.
	Metric 4:	Test Substance Stability	Medium	Minimal details on test substance preparation and no details on storage were reported

Domain 3: Test Conditions

Details

Study Citation:				Products of the gas-phase reactions of 1,3-butadiene with OH and NO3	
OECD Harmonized	radicals. Environmental Science & Technology 33(20):3586-3595. Photolysis in Air				
Template: HERO ID:	1742345				
HERO ID.	1742343				
ъ :			VALUATION		
Domain	Metric 5:	Metric Test Method Suitability	Rating	Comments The test method was suitable for the test substance.	
	Metric 6:	Testing Conditions	High Low	Minimal details on test set up and apparatus were reporetd.	
	Metric 7:	Testing Conditions Testing Consistency	Medium	Test conditions were presumably consistent throughout the study and between study	
	Wictire 7.	resting Consistency	Wicdiani	groups.	
	Metric 8:	System Type and Design	N/A	Not applicable.	
Di 4. T+ Oi-					
Domain 4: Test Organis	sms Metric 9:	Outcome Assessment Methodology	N/A	Not applicable.	
	Metric 10:	Sampling Methods	N/A	Not applicable.	
	THE TO.	Samping Medicus	17/11	Tot application	
Domain 5: Outcome As	ssessment				
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology was appropriate for determining overall loss and products. Rates were not determined.	
	Metric 12:	Test Substance Purity	High	Sampling methods were described and appropriate, frequency was acceptable for the reported endpoints.	
Domain 6: Confounding	a/Variable Central				
Domain o. Comounding	Metric 13:	Confounding Variables	High	Uncertainty in measurements and variability were explicitly addressed through appropri	
			· ·	ate statistical methods.	
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Not applicable.	
Domain 7: Data Present	tation and Analysis				
Domain 7. Data Mescil	Metric 15:	Data Reporting	Medium	The analytical method was appropriate; extraction efficiency and limits of detection	
	MICHICITY.	Data Reporting	Medium	were not reported. Product detection units were not reported.	
	Metric 16:	Statistical Methods and	N/A	Statistical and kinetic calculations were not conducted.	
		Kinetic Calculations			
Domain 8: Other					
Joinani 8: Other	Metric 17:	Verification or Plausibility of	Low	The results deviated significantly from previously reported product yields.	
	MEUIC 1/.	Results	LOW	The results deviated significantly from previously reported product yields.	
	Metric 18:	OSAR Models	N/A	Not applicable.	

Overall Quality Determination Medium

Study Citation: Tuazon, E. C., Alvarado, A., Aschmann, S. M., Atkinson, R., Arey, J. (1999). Products of the gas-phase reactions of 1,3-butadiene with OH and NO3

radicals. Environmental Science & Technology 33(20):3586-3595.

Not Reported; NR; NR

OECD Harmonized

Template:

Photolysis in Air

HERO ID: 1742345

Reference Substance Results, Percent Degrada-

Results Remarks, Sample time Results, Results Not Reported; NR; Not Reported

tion Results and Standard Deviation Results

Details

EXTRACTION	RACTION	
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Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	None; Experimental, NO3 radical, products reported, % loss degradation reported; None
Solvent, Reactivity, Storage, Stability	NA; NR; NR; NR
Radiolabel, Source, State, Purity	NA; Aldrich Chemical Co.; NR; >/= 99.0%
Duration and Test Temperature	NR; 298 ± 2 K
Light Source, Intensity, and additional light de-	Two parallel banks of black lamps; NR; 20% maximum light intensity used; NR
tails Source Wavelength Lower and Upper	300; NR
Test Details and Control	NO3 radicals generated by thermal decomposition of N2O5; NR
Initial Concentration, Reference	5.7 - 6.0E10^13 molecule/cm^3; NR
Compound	
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; NR; NR
Indirect Type Results, Indirect Rate	NO3 radicals; NR; NR
Constant Lower and Upper	
Method Details Results and Products	7500 L Teflon chamber at ~5% relative humidity, samples analyzed by GC-FID; Ratio: Acrolein (0.045), HCHO (0.065), furan (0.014), organic
Details Results	nitrates (0.63 Å \pm 0.15), and R(ONO2)(OONO2) species (0.08 â \in " 0.16)
Parameter Value and Parameter Results	Not Reported; Not Reported

		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified by name.
Metric 2:	Test Substance Purity	High	The test substance source and purity were reported.
Domain 2: Test Design			
Metric 3:	Study Controls	Medium	Dark controls were not explicitly included.
Metric 4:	Test Substance Stability	Medium	Minimal details on test substance preparation and no details on storage were reported
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
Metric 6:	Testing Conditions	Low	Minimal details on test set up and apparatus were reporetd.

		continu	ıed from previous p	page
Study Citation: OECD Harmonized		nmental Science & Technology 33(20):3586		Products of the gas-phase reactions of 1,3-butadiene with OH and NO3
Template:	1740045			
HERO ID:	1742345			
			EVALUATION	
Domain	36.1.5	Metric	Rating	Comments
	Metric 7:	Testing Consistency	Medium	Test conditions were presumably consistent throughout the study and between study groups.
	Metric 8:	System Type and Design	N/A	Not applicable.
Domain 4: Test Organis	eme			
Domain 4. Test Organis	Metric 9:	Outcome Assessment Methodology	N/A	Not applicable.
	Metric 10:	Sampling Methods	N/A	Not applicable.
	11101110 101	Samping meaneds	1,1,1	1.00 approximation
Domain 5: Outcome As	ssessment			
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology was appropriate for determining overall loss and products. Rates were not determined.
	Metric 12:	Test Substance Purity	High	Sampling methods were described and appropriate, frequency was acceptable for the reported endpoints.
Domain 6: Confoundin	g/Variable Control			
Domain o. Comounain	Metric 13:	Confounding Variables	High	Uncertainty in measurements and variability were explicitly addressed through appropriate statistical methods.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Not applicable.
Domain 7: Data Presen	tation and Analysis			
Domain 7. Dan Hosell	Metric 15:	Data Reporting	Medium	The analytical method was appropriate; extraction efficiency and limits of detection were not reported. Product detection units were not reported.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	Statistical and kinetic calculations were not conducted.
Domain 8: Other			_	
	Metric 17:	Verification or Plausibility of Results	Low	The results deviated significantly from previously reported product yields for most products except organic nitrates.
	Metric 18:	QSAR Models	N/A	Not applicable.

Overall Quality Determination Mealum

Study Citation: U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.

OECD Harmonized

Iarmonized Photolysis in Air

Template:

EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-butadiene			
Confidentiality, Type, Guideline	Not Reported; Not Reported			
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported			
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported			
Duration and Test Temperature	Not Reported; 25 deg C			
Light Source, Intensity, and additional light de-	Not Reported; Not Reported			
tails	N. a December de N. a December d			
Source Wavelength Lower and Upper	Not Reported; Not Reported			
Test Details and Control	Not Reported; Not Reported			
Initial Concentration, Reference Compound	Not Reported Not Reported; Not Reported			
Substance Wavelength Lower and Upper	Not Reported; Not Reported			
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported			
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported			
Method Details Results and Products Details Results	Not Reported; Not Reported			
Parameter Value and Parameter Results	Not Reported; Not Reported			
Reference Substance Results, Percent Degradation Results and Standard	Not Reported; Not Reported; Not Reported			
Deviation Results Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Degradation product from reaction with ozone: Acrolein			

			EVALUATIO	N	
Domain		Metric	Rating	Comments	
Domain 1: Test Substance					
Metri	ic 1:	Test Substance Identity	High	The test substance was identified.	
Metri	ic 2:	Test Substance Purity	N/A	This metric is not applicable to this study type.	
Domain 2: Test Design					
Metri	ic 3:	Study Controls	N/A	This metric is not applicable to this study type.	
Metri	ic 4:	Test Substance Stability	N/A	This metric is not applicable to this study type.	
Domain 3: Test Conditions					
Metri	ic 5:	Test Method Suitability	N/A	This metric is not applicable to this study type.	
Continued on next page					

		continu	ied from pre	vious page		
Study Citation:	, ,	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.				
OECD Harmonized	Photolysis in Air					
Template: HERO ID:	2454					
пекотр:	3454					
- ·			EVALUATIO			
Domain	16.1.6	Metric	Rating	Comments		
	Metric 6:	Testing Conditions	N/A	This metric is not applicable to this study type.		
	Metric 7:	Testing Consistency	N/A	This metric is not applicable to this study type.		
	Metric 8:	System Type and Design	N/A	This metric is not applicable to this study type.		
Domain 4: Test Organis	sms					
· ·	Metric 9:	Outcome Assessment Methodology	N/A	This metric is not applicable to this study type.		
	Metric 10:	Sampling Methods	N/A	This metric is not applicable to this study type.		
D : 5 0						
Domain 5: Outcome As		T (C) (II (')	NT/A			
	Metric 11:	Test Substance Identity	N/A	This metric is not applicable to this study type.		
	Metric 12:	Test Substance Purity	N/A	This metric is not applicable to this study type.		
Domain 6: Confoundin	g/Variable Control					
	Metric 13:	Confounding Variables	N/A	This metric is not applicable to this study type.		
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric is not applicable to this study type.		
		Exposure				
Domain 7: Data Presen	tation and Analysis					
	Metric 15:	Data Reporting	N/A	This metric is not applicable to this study type.		
	Metric 16:	Statistical Methods and	N/A	This metric is not applicable to this study type.		
		Kinetic Calculations		The moute is not appreciate to any study type.		
Domain 8: Other						
	Metric 17:	Verification or Plausibility of	N/A	This metric is not applicable to this study type.		
	Metric 18:	Results QSAR Models	N/A	This metric is not applicable to this study type.		
0 110 11			TT! 1			
Overall Quali	ty Determin	nation	High			

Study Citation: U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene. Photolysis in Air

OECD Harmonized Template:

HERO ID:

3454

E	EXTRACTION

	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, Type, Guideline	Not Reported; Not Reported
Solvent, Reactivity, Storage, Stability	Not Reported; Not Reported; Not Reported
Radiolabel, Source, State, Purity	Not Reported; Not Reported; Not Reported
Duration and Test Temperature	Not Reported; 25 deg C
Light Source, Intensity, and additional light de-	Not Reported; Not Reported
tails Source Wavelength Lower and Upper	Not Reported; Not Reported
Test Details and Control	Not Reported; Not Reported
Initial Concentration, Reference Compound	Not Reported Not Reported; Not Reported
Substance Wavelength Lower and Upper	Not Reported; Not Reported
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	Not Reported; Not Reported
Indirect Type Results, Indirect Rate	Not Reported; Not Reported
Constant Lower and Upper	
Method Details Results and Products	Not Reported; Not Reported
Details Results Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degradation Results and Standard	Not Reported; Not Reported
Deviation Results Results Remarks, Sample time Results, Results Details	Not Reported; Not Reported; Degradation product from reaction with ozone: Acrolein

			EVALUATIO	N	
Domain		Metric	Rating	Comments	
Domain 1: Test Substan	nce				
	Metric 1:	Test Substance Identity	High	The test substance was identified.	
	Metric 2:	Test Substance Purity	N/A	This metric is not applicable to this study type.	
Domain 2: Test Design					
	Metric 3:	Study Controls	N/A	This metric is not applicable to this study type.	
	Metric 4:	Test Substance Stability	N/A	This metric is not applicable to this study type.	
Domain 3: Test Condit	ions				
	Metric 5:	Test Method Suitability	N/A	This metric is not applicable to this study type.	
	Metric 6:	Testing Conditions	N/A	This metric is not applicable to this study type.	
	Metric 7:	Testing Consistency	N/A	This metric is not applicable to this study type.	
	Continued on next page				

Study Citation: OECD Harmonized Template: U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.

Photolysis in Air

Template: HERO ID:	3454			
			EVALUATIO	N
Domain		Metric	Rating	Comments
	Metric 8:	System Type and Design	N/A	This metric is not applicable to this study type.
Domain 4: Test Org	anisms			
_	Metric 9:	Outcome Assessment Methodology	N/A	This metric is not applicable to this study type.
	Metric 10:	Sampling Methods	N/A	This metric is not applicable to this study type.
Domain 5: Outcome	e Assessment			
	Metric 11:	Test Substance Identity	N/A	This metric is not applicable to this study type.
	Metric 12:	Test Substance Purity	N/A	This metric is not applicable to this study type.
Domain 6: Confour	nding/Variable Control			
	Metric 13:	Confounding Variables	N/A	This metric is not applicable to this study type.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric is not applicable to this study type.
		Exposure		
Domain 7: Data Pre	esentation and Analysis			
	Metric 15:	Data Reporting	N/A	This metric is not applicable to this study type.
	Metric 16:	Statistical Methods and	N/A	This metric is not applicable to this study type.
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	High	The reported values were consistent with related physical chemical properties.
	Metric 18:	Results QSAR Models	N/A	This metric is not applicable to this study type.
Overall Qua	ality Determin	ation	High	

Study Citation: Vimal, D. (2008). Laboratory investigations of the hydroxyl radical-initiated oxidation of atmospheric volatile organic compounds. ProQuest Dissertations

and Theses Doctoral Dissertation:213. Photolysis in Air

OECD Harmonized Template:

HERO ID: 5699949

EXT	$\Gamma \mathbf{R} \Delta$	C	ГT	N	N

EXTRACTION				
Parameter	Data			
CASRN and Test Material	Not Reported; 1,3-Butadiene			
Confidentiality, Type, Guideline	No; experimental; other: Gas-phase reaction of OH radical and 1,3-butadiene using a discharge flow technique			
Solvent, Reactivity, Storage, Stability	NR; NR; NR			
Radiolabel, Source, State, Purity	NR; Sigma-Aldrich; Not Reported; 99% Notes: Reagent mixtures prepared as 0.08-0.4% 1,3-butadiene)			
Duration and Test Temperature	Not Reported; 263 - 423 K (reaction temperatures controlled and monitored); total pressures 1-6 Torr			
Light Source, Intensity, and additional light details	OH radicals were produced by the F + H2O OH + HF reaction or the H + NO2 OH + NO reaction.; not applicable; Flow tube reactor with photomultiplier using National Instruments LabView hardware/software environment user interface Ctrdaq_e.vi designed by Dr. Drew L'Esperance. Reactor: jacketed 1 m long, 2.54 cm diameter pyrex glass tube connected to a Haolocarbon wax coated aluminum detection chamber evacuated by a mechanical pump (average velocity: ca. 10 m/s)			
Source Wavelength Lower and Upper	not applicable; not applicable			
Test Details and Control	OH concentrations below 3E11 molecules/cm3; experiments were performed with either resonance fluorescence or laser induced fluorescence detection of the OH radicals; laser-induced fluorescence detection of OH: minimum detectable OH concentration of approximately 2E7 molecules cm-3 (S/N=1; 10 s integration time); resonance fluorescence detection of OH: minimum detectable OH concentration of approximately 1E9 molecules cm-3 (background signal 300-400 counts/s, S/N=1; 10 s integration time); not reported			
Initial Concentration, Reference	Test concentrations ranged from 1.16 to 44.57 10^11 cm-3; Not reported			
Compound				
Substance Wavelength Lower and Upper	not reported; not reported			
Direct Quantum Yield Results, Direct Half Life	not reported; Not Reported; Not Reported			
by Loss Lower and Upper				
Indirect Type Results, Indirect Rate	bimolecular rate constant k^II OH + 1,3-Butadiene (10^{-11} cm3 molecule-1 s-1); 3.15 ± 0.28 (at 423 K); 8.57 ± 0.42 (at 263 K)			
Constant Lower and Upper Method Details Results and Products Details Results Parameter Value and Parameter Results	Pseudo-first-order decay rates: slope of log OH fluorescence signal versus reaction distance for given reagent concentration under plug flow approximation; first-order decay rates were corrected for axial diffusion and OH loss; bimolecular rate constants (k1^I) at variable pressures and temperatures calculated from weighted linear least-squares fit of k^I versus 1,3-butadiene concentration.; Based on results evaluating the isotopic effect, indicates that OH addition dominates the mechanism for photooxidation of 1,3-butadiene and H-abstraction is not occurring at a significant rate under these experimental conditions Not Reported; Not Reported			
Reference Substance Results, Percent Degrada-	kinetic isotope effect at a temperature of 363 K and pressure of 1 Torr (kII(D) = $(4.79 \pm 0.4) \times 10$ -11 cm3 molecule-1 s-1; kII(H) = $(4.75 \pm 0.3) \times 10$ -11 cm3 molecule-1 s			
tion Results and Standard	10-11 cm3 molecule-1 s-1); OH + 1,3-butadiene-d6 at 300K (1,3-butadiene-d6: $2.2-14.24 \times 10^{11}$ cm-3) k^II = $6.94 \pm 0.38 \times 10^{11}$ cm3 molecule-1			
Deviation Results Results Remarks, Sample time Results, Results Details	s-1 (value based on 15 experiments); not reported; reported with values: \pm uncertainties represent 2 standard deviations Arrhenius expression: kII (T) = $(7.23 \pm 1.2) \times 10$ -12 exp((664 \pm 49/T)) cm3 molecule-1 s-1; Not Reported; At 283K (1,3-butadiene: 1.53-16.89x10^11 cm-3) k^II = 7.68 ± 0.30 x10^-11 cm3 molecule-1 s-1 (value based on 13 experiments) At 300K, 2 Torr (1,3-butadiene: 2.24-20.81x10^11 cm-3) k^II = 6.96 ± 0.68 x10^-11 cm3 molecule-1 s-1 (value based on 17 experiments) At 300K, 3 Torr (1,3-butadiene: 1.91-24.21x10^11 cm-3) k^II = 7.01 ± 0.45 x10^-11 cm3 molecule-1 s-1 (value based on 16 experiments) At 300K, 5 Torr (1,3-butadiene: 2.41-24.7x10^11 cm-3) k^II = 6.99 ± 0.28 x10^-11 cm3 molecule-1 s-1 (value based on 54 experiments)			
	ENVAL MARINON			

EVALUATION

Continued on next page ...

Study Citation: Vimal, D. (2008). Laboratory investigations of the hydroxyl radical-initiated oxidation of atmospheric volatile organic compounds. ProQuest Dissertations and Theses Doctoral Dissertation:213. Photolysis in Air

OECD Harmonized

Template:

HERO ID:	5699949			
]	EVALUATIO	N
Domain		Metric	Rating	Comments
Domain		Metric	Rating	Comments
Domain 1: Test Substa				
	Metric 1:	Test Substance Identity	High	The test substance was identified clearly.
	Metric 2:	Test Substance Purity	High	The source and purity of the test substance were reported.
Domain 2: Test Design	1			
Domain 2. Test Design	Metric 3:	Study Controls	High	Blanks were run and accounted for in the data.
	Metric 4:	Test Substance Stability	High	The test substance preparation was reported.
Domain 3: Test Condi		T . M . L . L C . L . L . L . L . L . L . L .	TT: 1	
	Metric 5:	Test Method Suitability	High	The test method was suitable.
	Metric 6:	Testing Conditions	High Madium	Testing conditions were monitored, reported, and appropriate for the method.
	Metric 7: Metric 8:	Testing Consistency System Type and Design	Medium High	Variable [He], [1,3-butadiene], and number of experiments run at several temperatures.
	Metric 6.	System Type and Design	nigii	The system type and design were appropriate.
Domain 4: Test Organ	isms			
C	Metric 9:	Outcome Assessment Methodology	N/A	This metric is not applicable to the study type.
	Metric 10:	Sampling Methods	N/A	This metric is not applicable to the study type.
Domain 5: Outcome A		T . C	TT: 1	
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed the intended outcome of interest.
	Metric 12:	Test Substance Purity	N/A	This metric is not applicable to this study type.
Domain 6: Confoundin	ng/Variable Control			
	Metric 13:	Confounding Variables	High	Reported variability or uncertainty was not likely to influence the outcome assessment.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric is not applicable to the study type.
		Exposure		
Domain 7: Data Preser	ntation and Analysis			
Domain 7. Data 1 16861	Metric 15:	Data Reporting	High	Data reporting was appropriate.
	Metric 16:	Statistical Methods and	High	Kinetic calculations were described and address the data.
	Medic 10.	Kinetic Calculations	i ii gii	Tribote edicalations were described and address the data.
Domain 8: Other				
Domain o. Other	Metric 17:	Verification or Plausibility of	High	The study results were reasonable and compared to previously reported literature values
		Results QSAR Models	_	
	Metric 18:	QSAR Models	N/A	This metric is not applicable to the study type.

Study Citation: Vimal, D. (2008). Laboratory investigations of the hydroxyl radical-initiated oxidation of atmospheric volatile organic compounds. ProQuest Dissertations

and Theses Doctoral Dissertation:213. Photolysis in Air

OECD Harmonized Template:

		EVALUATION		
Domain	Metric	Rating	Comments	
Overall Quality Determination		High		

Study Citation: NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.

OECD Harmonized

nized Hydrolysis

Template:

HERO ID: 6628926

	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	none; not specified; Not Reported: not specified
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Buffer, Test Temperature, Number of Replicates	NR; NR; NR
Positive Controls and Negative Controls	Positive: NR; Negative: NR
pH and Duration	NR; NR
Sampling Frequency and Test Setup	NR; NR
Concentration	Not Reported
Analytical Method, Analytical Details, and	NR; NR; NR
Statistics Transformation Products	NR
Reference Substance and Reference	NR; NR
Substance Results Percent Recovery, Hydrolysis Rate Constant, and Half-life	NR; NR; NR
Results Remarks	Not expected to undergo hydrolysis in the environment due to a lack of hydrolyzable functional groups

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substa	ance			
	Metric 1:	Test Substance Identity	High	The test substance was identified.
	Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported in this secondary source.
Domain 2: Test Desig	n			
	Metric 3:	Study Controls	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 4:	Test Substance Stability	Medium	Details regarding this metric were not reported in this secondary source.
Domain 3: Test Condi	tions			
	Metric 5:	Test Method Suitability	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 6:	Testing Conditions	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 7:	Testing Consistency	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 8:	System Type and Design	Medium	Details regarding this metric were not reported in this secondary source.

Domain 4: Test Organisms

Study Citation: NCBI, (2020). PubChem database: compound summary: 1,3-butadiene. **OECD Harmonized** Hydrolysis **Template: HERO ID:** 6628926 **EVALUATION** Metric Domain Rating Comments Metric 9: Outcome Assessment Methodology N/A The metric is not applicable to the study. Metric 10: Sampling Methods N/A The metric is not applicable to the study. Domain 5: Outcome Assessment Test Substance Identity Metric 11: Medium Details regarding this metric were not reported in this secondary source. Metric 12: Test Substance Purity Medium Details regarding this metric were not reported in this secondary source. Domain 6: Confounding/Variable Control

Domain 7: Da	a Presentation	and	l Analysis	

Metric 13:

Metric 14:

Metric 15:	Data Reporting	Medium	Details regarding this metric were not reported in this secondary source.
Metric 16:	Statistical Methods and	Medium	Details regarding this metric were not reported in this secondary source.
	Kinetic Calculations		

Medium

N/A

Details regarding this metric were not reported in this secondary source.

The metric is not applicable to the study.

Domain 8: Other

Metric 17:	Verification or Plausibility of	Low	Results were limited to a qualitative assessment.
Metric 18:	Results OSAR Models	N/A	The meeting is not applicable to the study
Metric 18:	QSAR Models	IN/A	The metric is not applicable to the study.

Overall Quality Determination

Medium

Confounding Variables

Exposure

Health Outcomes Unrelated to

^{*} Related References: Primary source cited: Capel PD, Larson SJ; Chemosphere 30: 1097- 1107 (1995)

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized

:380-381. Photolysis in Water

Template:

HERO ID: 11779754

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	EATRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	no; calculation; EPA OTS 796.3700 (Direct Photolysis Rate in Water by Sunlight): NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Duration and Test Temperature	NR; NR
Light Source, Intensity, and additional light de-	NR; NR; NR
tails	NID, NID
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration and Reference Compound	NR NR; NR
Substance Wavelength Lower and Upper	NR; NR
Direct Quantum Yield Results, Direct Half Life by Loss Lower and Upper	NR; Indirect half-life = 1200 hours (50 days); Indirect half-life = 48000 hours (200 days)
Indirect Rate Constant Lower and Upper	NR; NR
Method Details Results and Products	NR; NR
Details Results	NID NID
Parameter Value and Parameter Results	NR; NR
Reference Compound, Reference	NR; NR; NR
Substance Results, Percent Degradation Results and Standard Deviation Results Results Remarks, Sample time Results, Results Details	Based on measured hydroxyl radical rate constant in water; NR; NR

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substa	ance			
	Metric 1:	Test Substance Identity	High	The test material was identified definitively.
	Metric 2:	Test Substance Purity	Medium	The source and purity of the test substance were not reported; however, the omissions were not likely to have a substantial impact on the study results.
Domain 2: Test Design	n			
	Metric 3:	Study Controls	Medium	Study controls were not reported and may affect the study results; however, the data are from a trusted secondary source.
	Metric 4:	Test Substance Stability	Medium	The test substance stability, homogeneity, preparation or storage conditions were not reported; however, these factors were not likely to influence the test substance or were not likely to have a substantial impact on study results.

Continued on next page ...

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

:380-381. Photolysis in Water **OECD Harmonized**

Template:

HERO ID: 11779754

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Cond	ditions			
	Metric 5:	Test Method Suitability	Medium	The test method was not reported; however, the data is from a trusted secondary source with reference to the source the calculation was based on.
	Metric 6:	Testing Conditions	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 7:	Testing Consistency	Medium	Testing conditions were not reported; however, the data are from a trusted secondary source.
	Metric 8:	System Type and Design	Medium	Equilibrium was not reported; however, the data are from a trusted secondary source.
Domain 4: Test Orga	nnisms			
<i>8</i> .	Metric 9:	Outcome Assessment Methodology	N/A	This metric does not apply to this study type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome				
	Metric 11:	Test Substance Identity	High	The outcome of interest was reported.
	Metric 12:	Test Substance Purity	Medium	The sampling method was not reported; however, the data are from a trusted secondary source.
Domain 6: Confound	ding/Variable Control			
	Metric 13:	Confounding Variables	Medium	Sources of variability and uncertainty in the measurements were not reported; however, the omissions were not likely to have a substantial impact on study results.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Pres	sentation and Analysis	•		
Domain 7. Data 110s	Metric 15:	Data Reporting	Medium	Data reporting was limited, the analytical method was not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	Medium	Kinetic and calculation details were not reported; however, the information is presented in a trusted secondary source.
Domain 8: Other				
,	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.
Overall Oua	lity Determin	ation	Medium	
O TOTALL QUA			Micuidili	

^{*} Related References: Guesten, H et al 1981

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized

:380-381. Biodegradation in Water

half-lives.; NR

NR; NR

Template:

covery

HERO ID: 11779754

Results Mean Total Recovery and Results per Re-

D	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type, Guideline	No; Other; Calculation (scientific judgement); other: NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Blank and Control	NR; NR
Oxygen and Inoculum	Not specified; not specified: ground water
Duration, Parameter, System, and Sampling Frequency	NR; NR: NR
pH Adjusted and pH	NR; NR
Concentration	NR NR - NR NR NR
Composition and Test Temperature	NR; NR
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	NR; NR; NR
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	NR; NR; NR
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	NR; NR; NR
Results Remarks and Results Details	Ground water half-life: 336 hours (14 days) - 1344 hours (8 weeks); scientific judgement based on estimated aqueous aerobic biodegradation

		EVALUATIO	N
Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1	: Test Substance Identity	High	The test substance was identified definitively.
Metric 2	: Test Substance Purity	N/A	This metric is not applicable to the data type.
D 1 0 m . D 1			
Domain 2: Test Design			
Metric 3	: Study Controls	Low	Study controls were not reported and may affect the study results; however, the data are from a trusted secondary source.
Metric 4	: Test Substance Stability	N/A	This metric is not applicable to the data type.

Continued on next page ...

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized

:380-381. Biodegradation in Water

Template:

Metric Test Method Suitability Testing Conditions Testing Consistency System Type and Design Outcome Assessment Methodology Sampling Methods Test Substance Identity	Low Low N/A N/A N/A Medium	The test method was not reported and citations were not provided. Testing conditions were not reported and citations were not provided. This metric is not applicable to the data type. This metric is not applicable to the data type. The metric is not applicable to the data type. This metric does not apply to this study type.
Testing Conditions Testing Consistency System Type and Design Outcome Assessment Methodology Sampling Methods Test Substance Identity	Low N/A N/A N/A N/A	Testing conditions were not reported and citations were not provided. This metric is not applicable to the data type. This metric is not applicable to the data type. The metric is not applicable to the data type. This metric does not apply to this study type.
Testing Conditions Testing Consistency System Type and Design Outcome Assessment Methodology Sampling Methods Test Substance Identity	Low N/A N/A N/A N/A	Testing conditions were not reported and citations were not provided. This metric is not applicable to the data type. This metric is not applicable to the data type. The metric is not applicable to the data type. This metric does not apply to this study type.
Testing Consistency System Type and Design Outcome Assessment Methodology Sampling Methods Test Substance Identity	N/A N/A N/A N/A	This metric is not applicable to the data type. This metric is not applicable to the data type. The metric is not applicable to the data type. This metric does not apply to this study type.
Outcome Assessment Methodology Sampling Methods Test Substance Identity	N/A N/A N/A	This metric is not applicable to the data type. The metric is not applicable to the data type. This metric does not apply to this study type.
Outcome Assessment Methodology Sampling Methods Test Substance Identity	N/A N/A	The metric is not applicable to the data type. This metric does not apply to this study type.
Sampling Methods Test Substance Identity	N/A	This metric does not apply to this study type.
Sampling Methods Test Substance Identity	N/A	This metric does not apply to this study type.
Test Substance Identity		***
·	Medium	
·	Medium	
		The outcome of interest was reported; however, there was incomplete reporting of outcome assessment methods.
Test Substance Purity	N/A	This metric is not applicable to the data type.
ontrol		
Confounding Variables	Low	Confounding variables were not discussed.
Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
Exposure	1,11	This metric does not apply to this study type.
alysis		
_ -	Low	Data reporting was limited, basis for scientific judgement and estimations were not reported; however, the information is presented in a trusted secondary source.
Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type.
Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
QSAR Models	N/A	This metric does not apply to this study type.
	Statistical Methods and Kinetic Calculations Verification or Plausibility of Results QSAR Models	Statistical Methods and N/A Kinetic Calculations Verification or Plausibility of Low Results

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized

:380-381. Biodegradation in Water

Template:

HERO ID: 11779754

EXTRACTION	
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Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type, Guideline	No; Aqueous biodegradation; Calculation (scientific judgement); other: NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Blank and Control	NR; NR
Oxygen and Inoculum	Aerobic; not specified: unacclimated
Duration, Parameter, System, and Sampling Frequency	NR; NR: NR
pH Adjusted and pH	NR; NR
Concentration	NR NR - NR NR NR
Composition and Test Temperature	NR; NR
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	NR; NR; NR
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	NR; NR; NR
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	NR; NR; NR
Results Remarks and Results Details	Aerobic half-life: 168 hours (7 days) - 672 hours (4 weeks) (Aqueous biodegradation); scientific judgement.; NR
Results Mean Total Recovery and Results per Recovery	NR; NR

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Test Substan	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively.
	Metric 2:	Test Substance Purity	Medium	The source and purity of the test substance were not reported; however, the omissions were not likely to have a substantial impact on the study results.
Domain 2: Test Design				
	Metric 3:	Study Controls	Low	Study controls were not reported and citations were not provided; however, the data are from a trusted secondary source.
	Metric 4:	Test Substance Stability	Low	The test substance stability, homogeneity, preparation or storage conditions were not reported and citations were not provided; however, the data are from a trusted secondary source.

Continued on next page ...

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized

:380-381. Biodegradation in Water

Template:

		1	EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 3: Test Cond	itions			
	Metric 5:	Test Method Suitability	Low	The test method was not reported and citations were not provided.
	Metric 6:	Testing Conditions	Low	Testing conditions were not reported and citations were not provided.
	Metric 7:	Testing Consistency	N/A	This metric does not apply to this data type.
	Metric 8:	System Type and Design	Low	Equilibrium was not reported; however, the data are from a trusted secondary source.
Domain 4: Test Orgai	nisms			
Č	Metric 9:	Outcome Assessment Methodology	Low	The inoculum and source were not reported and citations were not provided; however, the data are from a trusted secondary source.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome	Assessment			
Domain 3. Outcome	Metric 11:	Test Substance Identity	Medium	The outcome of interest was reported; however, there was incomplete reporting of outcome assessment methods.
	Metric 12:	Test Substance Purity	Low	The sampling method was not reported and citations were not provided; however, the data are from a trusted secondary source.
Domain 6: Confound	ing/Variable Control			
Domain o. Comouna	Metric 13:	Confounding Variables	N/A	This metric does not apply to this study type.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.
Domain 7: Data Prese	entation and Analysis			
	Metric 15:	Data Reporting	Low	Data reporting was limited, basis for scientific judgement and estimations were not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.
Overall Oual	lity Determin	ation	Low	

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

:380-381. Biodegradation in Water **OECD Harmonized**

Template:

	EATRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type, Guideline	No; Other; Calculation (scientific judgement); other: NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Blank and Control	NR; NR
Oxygen and Inoculum	Not specified; other:: surface water
Duration, Parameter, System, and Sampling Frequency	NR; NR: NR
pH Adjusted and pH	NR; NR
Concentration	NR NR - NR NR NR
Composition and Test Temperature	NR; NR
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	NR; NR; NR
Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	NR; NR; NR
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	NR; NR; NR
Results Remarks and Results Details	Surface water half-life: 168 hours (7 days) - 672 hours (4 weeks); based on estimated aerobic biodegradation half-lives.; NR
Results Mean Total Recovery and Results per Recovery	NR; NR

Rating Intity High rity N/A	Comments The test substance was identified definitively. This metric is not applicable to the data type.
-	·
-	·
rity N/A	This metric is not applicable to the data type.
Low	Study controls were not reported and citations were not provided; however, the data are from a trusted secondary source.
bility N/A	This metric is not applicable to the data type.
bility Low	The test method was not reported and citations were not provided.
Low	Testing conditions were not reported and citations were not provided.
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		continu	ed from previou	s page		
Study Citation:	Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene. :380-381. Biodegradation in Water					
OECD Harmonized						
Template:						
HERO ID:	11779754					
		E	VALUATION			
Domain		Metric	Rating	Comments		
	Metric 7:	Testing Consistency	N/A	This metric does not apply to this data type.		
	Metric 8:	System Type and Design	N/A	This metric does not apply to this data type.		
Domain 4: Test Organis	sms					
Ü	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to the data type.		
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.		
Domain 5: Outcome As						
	Metric 11:	Test Substance Identity	Medium	The outcome of interest was reported; however, there was incomplete reporting of outcome assessment methods.		
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to the data type.		
Domain 6: Confounding	g/Variable Control					
Domain o. Comounaing	Metric 13:	Confounding Variables	Low	Confounding variables were not discussed.		
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.		
		Exposure				
Domain 7: Data Present	tation and Analysis					
	Metric 15:	Data Reporting	Medium	Data reporting was limited, basis for scientific judgement and estimations were not reported; however, the information is presented in a trusted secondary source.		
	Metric 16:	Statistical Methods and	N/A	This metric does not apply to this study type.		
		Kinetic Calculations				
Domain 8: Other						
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was no possible.		
	Metric 18:	OSAR Models	N/A	This metric does not apply to this study type.		

Overall Quality Determination Medium **Study Citation:** Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized

:380-381. Biodegradation in Water

Template:

covery

	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type, Guideline	No; Aqueous biodegradation; Calculation (scientific judgement); other: NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Blank and Control	NR; NR
Oxygen and Inoculum	Anaerobic; not specified: unacclimated
Duration, Parameter, System, and Sampling Frequency	NR; NR: NR; NR
pH Adjusted and pH	NR; NR
Concentration	NR NR - NR NR NR
Composition and Test Temperature	NR; NR
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	NR; NR; NR
Results Details Method, Results per Degradation Parameter, and	NR; NR; NR
Direct Quantum Yield Results Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	NR; NR; NR
Results Remarks and Results Details	Anaerobic half-life: 672 hours (28 days) -2688 hours (16 weeks) (Aqueous biodegradation); scientific judgement based upon estimated aqueous aerobic biodegradation half-lives.; NR
Results Mean Total Recovery and Results per Re-	NR; NR

		EVALUATIO:	N
Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1	: Test Substance Identity	High	The test substance was identified definitively.
Metric 2	: Test Substance Purity	Medium	The source and purity of the test substance were not reported; however, the omissions were not likely to have a substantial impact on the study results.
Domain 2: Test Design			
Metric 3	: Study Controls	Low	Study controls were not reported and citations were not provided; however, the data are from a trusted secondary source.
Metric 4	: Test Substance Stability	Low	The test substance stability, homogeneity, preparation or storage conditions were not reported and citations were not provided; however, the data are from a trusted secondary source.

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized

:380-381. Biodegradation in Water

Template: HERO ID:

11770754

HERO ID:	11779754			
		1	EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 3: Test Condi	itions			
Bomain 3. Test Come.	Metric 5:	Test Method Suitability	Low	The test method was not reported and citations were not provided; however, the data are from a trusted secondary source.
	Metric 6:	Testing Conditions	Low	Testing conditions were not reported and citations were not provided.
	Metric 7:	Testing Consistency	N/A	This metric does not apply to this data type.
	Metric 8:	System Type and Design	Low	Equilibrium was not established or reported; however, the data are from a trusted secondary source.
Domain 4: Test Orgar	nisms			
Domain 1. Test Organ	Metric 9:	Outcome Assessment Methodology	Low	The inoculum and source were not reported and citations were not provided; however, the data are from a trusted secondary source.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
D : 5 O :				
Domain 5: Outcome A	Assessment Metric 11:	Test Substance Identity	Medium	The outcome of interest was reported; however, there was incomplete reporting of outcome assessment methods.
	Metric 12:	Test Substance Purity	Low	The sampling method was not reported and citations were not provided; however, the data are from a trusted secondary source.
Domain 6: Confoundi	ing/Variable Control			
Domain o. Comound	Metric 13:	Confounding Variables	N/A	This metric does not apply to the data type.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		This metric does not apply to this stady types
Domain 7: Data Prese	entation and Analysis			
Domain 7. Data 11050	Metric 15:	Data Reporting	Low	Data reporting was limited, basis for scientific judgement and estimations were not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.
Overall Qual	lity Determin	nation	Low	

Study Citation:

NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.

OECD Harmonized

Biodegradation in Water

Template:

EXTRACTION				
Parameter	Data			
CASRN and Test Material	106-99-0; 1,3-Butadiene			
Confidentiality, EndPoint, Type,	None; other; Experimental; other			
Guideline Solvent, Reactivity, Storage, Stability	NR; NR; NR			
Radiolabel, Source, State, Purity	NR; NR; NR			
Blank and Control	Not reported; Not reported			
Oxygen and Inoculum	aerobic/anaerobic; not specified: Not reported			
Duration, Parameter, System, and	Not reported; Not Reported: Not reported; Not reported			
Sampling Frequency				
pH Adjusted and pH	Not Reported; Not reported			
Concentration	Not Reported			
Composition and Test Temperature	Aerobic waters/anaerobic waters; Not reported			
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	Not reported; Not reported; Not Reported; Not reported			
Results Details Method, Results per Degradation Parameter, and	Not reported; Aerobic biodegradation half-life; anaerobic biodegradation half-life; Not Reported			
Direct Quantum Yield Results				
Results Value, Results Standard Deviation, Re-	7 days; 28 days; Not reported; Not reported			
sults Sample Time, and Results Reference Sub-				
stance Compartments				
Results Remarks and Results Details	Not reported; Not reported			
Results Mean Total Recovery and Results per Recovery	Not reported; Not reported			

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substar	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified clearly.
	Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported in this secondary source.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Limited data is presented in this secondary source.
	Metric 4:	Test Substance Stability	Medium	Limited data is presented in this secondary source.
Domain 3: Test Conditi	ions			
	Metric 5:	Test Method Suitability	Medium	Limited data is presented in this secondary source.
			Continued on next page	

		continu	ied from previous	page
Study Citation:	NCBI, (2020). P	PubChem database: compound summary: 1,	3-butadiene.	
OECD Harmonized	Biodegradation in Water			
Template:				
HERO ID:	6628926			
		F	EVALUATION	
Domain		Metric	Rating	Comments
	Metric 6:	Testing Conditions	Medium	Limited data is presented in this secondary source.
	Metric 7:	Testing Consistency	Medium	Limited data is presented in this secondary source.
	Metric 8:	System Type and Design	Medium	Limited data is presented in this secondary source.
Domain 4: Test Organi	sms			
C	Metric 9:	Outcome Assessment Methodology	Low	Limited data is presented in this secondary source.
	Metric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome A	ssessment			
	Metric 11:	Test Substance Identity	N/A	The intended outcome is reported for the target substance.
	Metric 12:	Test Substance Purity	Medium	Limited data is presented in this secondary source.
Domain 6: Confoundin	ug/Variable Control			
Domain o. Comounam	Metric 13:	Confounding Variables	Medium	Limited data is presented in this secondary source.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric is not applicable to this type of study.
	Wietrie 11.	Exposure	1771	This metre is not appreador to this type of study.
Domain 7: Data Presen	ntation and Analysis			
	Metric 15:	Data Reporting	Medium	Limited data is presented in this secondary source.
	Metric 16:	Statistical Methods and	Medium	Limited data is presented in this secondary source.
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric is not applicable to this type of study.
Overall Quali	ty Dotormii	nation	Medium	
Cycram Quan	ij Determin	iuuvii	Micuiuiii	

^{*} Related References: Primary source cited: Capel PD, Larson SJ; Chemosphere 30: 1097- 1107 (1995)

Study Citation: NCBI, (2020). PubChem database: compound summary: 1,3-butadiene. Biodegradation in Water

OECD Harmonized **Template:**

HERO ID: 6628926

FXTRACTION

Parameter	Data EXTRACTION
-	
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, EndPoint, Type,	None; ready biodegradability; Experimental; OECD Guideline 301 D (Ready Biodegradability: Closed Bottle Test): Similar to OECD 301D
Guideline Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR
Blank and Control	Not reported; Not reported
Oxygen and Inoculum	aerobic; not specified: sludge inoculum at 1 drop/liter
Duration, Parameter, System, and	4 weeks; not specified: Not reported; Not reported
Sampling Frequency	N. d. D. a. and d. N. d. annuald. d
pH Adjusted and pH	Not Reported; Not reported
Concentration	2.06 - 4.95 mg/L
Composition and Test Temperature	Not reported; Not reported
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	Not reported; Not reported; Not Reported; Not reported
Results Details Method, Results per Degradation	Not reported; Theoretical BOD; Not Reported
Parameter, and	
Direct Quantum Yield Results	
Results Value, Results Standard Deviation, Re-	4%; Not reported; Not reported
sults Sample Time, and Results Reference Sub-	
stance Compartments Results Remarks and Results Details	Not reported; Not reported
Results Mean Total Recovery and Results per Recovery	Not reported; Not reported

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substa	nce			
	Metric 1:	Test Substance Identity	High	The test substance was identified clearly.
	Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported in this secondary source.
Domain 2: Test Design	1			
	Metric 3:	Study Controls	Medium	Limited data is presented in this secondary source.
	Metric 4:	Test Substance Stability	Medium	Limited data is presented in this secondary source.
Domain 3: Test Condit	ions			
	Metric 5:	Test Method Suitability	High	Reported as similar to an OECD Guideline study.
	Metric 6:	Testing Conditions	Medium	Limited data is presented in this secondary source.
	Metric 7:	Testing Consistency	Medium	Limited data is presented in this secondary source.
			Continued on next page	

Study Citation: NCBI, (2020). PubChem database: compound summary: 1,3-butadiene. **OECD Harmonized** Biodegradation in Water **Template: HERO ID:** 6628926 **EVALUATION** Metric Domain Rating Comments Metric 8: System Type and Design High Reported as similar to an OECD Guideline study. Domain 4: Test Organisms Metric 9: Outcome Assessment Methodology Medium Reported as similar to an OECD Guideline study using a sludge inoculum. Metric 10: Sampling Methods N/A The metric is not applicable to the study type. Domain 5: Outcome Assessment Metric 11: Test Substance Identity High The intended outcome is reported for the target substance. Metric 12: Test Substance Purity Medium Limited data is presented in this secondary source. Domain 6: Confounding/Variable Control Metric 13: Confounding Variables Medium Limited data is presented in this secondary source. Metric 14: Health Outcomes Unrelated to N/A This metric is not applicable to this type of study. Exposure Domain 7: Data Presentation and Analysis Metric 15: **Data Reporting** Medium Limited data is presented in this secondary source. Metric 16: Statistical Methods and Medium Limited data is presented in this secondary source. Kinetic Calculations

Overall Quality Determination

Metric 17:

Metric 18:

Verification or Plausibility of

Results

QSAR Models

Domain 8: Other

Medium

Medium

N/A

Due to limited information, evaluation of the reasonableness of the study results was not

This metric is not applicable to this type of study.

^{*} Related References: NITE; Chemical Risk Information Platform (CHRIP). Biodegradation and Bioconcentration. Tokyo, Japan: Natl Inst Tech Eval. Available from, as of Mar 9, 2015: http://www.safe.nite.go.jp/english/db.html

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized

:380-381. Biodegradation in Soil

Template:

HERO ID: 11779754

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type, Guideline	no; other; Calculation (scientific judgement); other: NR
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Oxygen, pH, and CEC	NR; NR; NR
Test Type, Test Temperature, and Test Details	not specified; NR; NR
Soil Type, Clay Silts and Organic Carbon, and Bulk Density	other; NR; NR
Soil Classification, Microbial Biomass, and Humidity	NR; NR: NR
Duration, Parameter, System, and	NR; NR; NR
Sampling Frequency	
Control and Blank	NR; NR
Concentration	NR NR - NR NR
Analytical Method, Analytical Details, and Results Per Degredation Parameter	NR; NR; NR
Results Remarks	Half-life: 168-672 hours (7 days-4weeks) in soil; scientific judgement based upon estimated aqueous aerobic biodegradation half-lives.
Results Value, Standard Deviation Results, Sam- ple Time Results, Reference Substance Results, and Reference Substance Compartment Results	NR; NR; NR; NR
Results Details	NR
Mean Total Recovery Results and Results Per Recovery	NR; NR

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Test Substa	ance			
	Metric 1:	Test Substance Identity	High	The test material was identified definitively.
	Metric 2:	Test Substance Purity	N/A	The metric is not applicable to the data type.
D : 0 T (D :				
Domain 2: Test Design				
	Metric 3:	Study Controls	Low	Study controls were not reported and may affect the study results; however, the data are from a trusted secondary source.
	Metric 4:	Test Substance Stability	N/A	The metric is not applicable to the data type.

Continued on next page ...

Study Citation: Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 1,3-butadiene.

OECD Harmonized

:380-381. Biodegradation in Soil

Template: HERO ID:

11779754

		I	EVALUATIO:	N
Domain		Metric	Rating	Comments
Domain 3: Test Condi	tions			
	Metric 5:	Test Method Suitability	Low	The test method was not reported and citations were not provided.
	Metric 6:	Testing Conditions	Low	The test conditions were not reported.
	Metric 7:	Testing Consistency	N/A	The metric is not applicable to the data type.
	Metric 8:	System Type and Design	N/A	The metric is not applicable to the data type.
Domain 4: Test Organ	isms			
C	Metric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to the data type.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Domain 5: Outcome A	Assessment			
Z chiam of Gueome i	Metric 11:	Test Substance Identity	Medium	The outcome of interest was reported; however, there was incomplete reporting of outcome assessment methods.
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to the data type.
Domain 6: Confoundi	ng/Variable Control			
Domain o. Comouna	Metric 13:	Confounding Variables	Medium	Confounding variables were not reported.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Prese	ntation and Analysis			
	Metric 15:	Data Reporting	Low	Data reporting was limited, basis for scientific judgement and estimations were not reported; however, the information is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was not possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.
Overall Qual	ity Determin	ation	Low	

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

OECD Harmonized

Template:

EXTRACTION

Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	no; experimental; experimental
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	NR; NR; NR Notes: NR
Test Method Details, Test Condition Details, and	Oxidation of 1,3-butadiene with 27 strains of propane-utilising bacteria; Bacteria was incubated in a 50% 1,3-butadiene/50% oxygen atmosphere
Test Consistency	at 30C.; Not Reported
Details	and an all annual in a
System Type Design	resting cell suspensions
Sampling Frequency and Sampling Details	Not Reported; Not Reported
Test Temperature	Not Reported
Results Details	Not Reported
Analytical Method and Analytical Details	Not Reported; Not Reported
Transformation Products, Statistics, and Kinetics	1,2-epoxybutene; Not Reported; Not Reported
Reference Substance and Reference Substance Results	Not Reported; Not Reported

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substance				
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively
· · · · · · · · · · · · · · · · · · ·	Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 2: Test Design				
	Metric 3:	Study Controls	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 3: Test Conditions	S			
	Metric 5:	Test Method Suitability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 6:	Testing Conditions	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 8:	System Type and Design	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 4: Test Organisms	S			
	Metric 9:	Outcome Assessment Methodology	High	The test organism was reported; more details may be in the source cited.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
		Com	tinued on next nego	

		***************************************	unueu mom previous	k-m2-
Study Citation:	ECB, (2002). E	uropean Union risk assessment report: 1,	,3-butadiene.	
OECD Harmonized	Miscellaneous			
Template:				
HERO ID:	5155560			
			EVALUATION	
Domain		Metric	Rating	Comments
Domain 5: Outcome A	ssessment			
	Metric 11:	Test Substance Identity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 6: Confounding	ng/Variable Control			
	Metric 13:	Confounding Variables	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Preser	ntation and Analysi	S		
	Metric 15:	Data Reporting	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 16:	Statistical Methods and	N/A	This metric does not apply to this study type
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 18:	Results QSAR Models	N/A	This metric does not apply to this study type.
Overall Quali	ity Determi	nation	Medium	

^{*} Related References: Cited secondary source Hou CT, Patel R, Laskin AI, Barnabe N, Barist I (1983). Epoxidation of short-chain alkenes by resting-cellsuspensions of propane-grown bacteria. Appl Environ Microbiol. 46; 171-177. [Not in HERO at the time of extraction].

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

Data

OECD Harmonized Template:

Parameter

HERO ID: 5155560

EXTRACTION

CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	no; experimental; experimental
Solvent, Reactivity, Storage, Stability	NR; NR; NR; NR

Radiolabel, Source, State, Purity
Test Method Details, Test Condition Details, and

Test Method Details, Test Condition Details,

Test Consistency Details Not Reported; Culture of Norcardia that were isolated from soil were grown at 25C with 1,-butadiene present in the headspace by 10-15% by volume.; Not Reported

System Type Design Not Reported

Sampling Frequency and Sampling Details Not Reported; Not Reported

Test Temperature Not Reported
Results Details Not Reported

Analytical Method and Analytical Details Not Reported; Not Reported

Transformation Products, Statistics, and Kinetics Degrades by several steps to give carbon dioxide and acetate. The stepwise intermediates were thought to be monoepoxide, beta, gamma-

unsaturated alpha-keto acid, acrylate, lactate, and pyruvate; Not Reported; Not Reported

Reference Substance and Reference

Substance Results

Not Reported; Not Reported

NR: NR: NR: NR Notes: NR

		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Test Substance			
Metric 1:	Test Substance Identity	High	The test substance was identified definitively
Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 2: Test Design			
Metric 3:	Study Controls	Medium	Details regarding this metric were not reported; more details may be in the source cited
Metric 4:	Test Substance Stability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 3: Test Conditions			
Metric 5:	Test Method Suitability	Medium	Details regarding this metric were not reported; more details may be in the source cited
Metric 6:	Testing Conditions	Medium	Details regarding this metric were not reported; more details may be in the source cited
Metric 7:	Testing Consistency	Medium	Details regarding this metric were not reported; more details may be in the source cited
Metric 8:	System Type and Design	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 4: Test Organisms			
Metric 9:	Outcome Assessment Methodology	High	The test organism was reported; more details may be in the source cited.
Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.

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

Template:

HERO ID:

5155560

Miscellaneous

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 5: Outcome Asses	ssment			
	Metric 11:	Test Substance Identity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
· · · · · · · · · · · · · · · · · · ·	Metric 12:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 6: Confounding/\	/ariable Control			
	Metric 13:	Confounding Variables	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Presentati	ion and Analysis	S		
	Metric 15:	Data Reporting	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 16:	Statistical Methods and	N/A	This metric does not apply to this study type
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Medium	Details regarding this metric were not reported; more details may be in the source cited.
		Results		
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.
Overall Quality	Determi	nation	Medium	

^{*} Related References: Cited secondary source Watkinson and Somerville 1975 [HERO ID 5349224]

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

Data

OECD Harmonized Template:

Parameter

HERO ID: 5155560

EXTRACTION

CASRN and Test Material 106-99-0; 1,3-Butadiene Confidentiality, Type, Guideline no; experimental; experimental

NR; NR; NR; NR Solvent, Reactivity, Storage, Stability

Radiolabel, Source, State, Purity NR; NR; NR; NR Notes: NR

Test Method Details, Test Condition Details, and

Test Consistency

Details System Type Design resting cell suspensions

Sampling Frequency and Sampling Details

Test Temperature Not Reported Results Details Not Reported

Analytical Method and Analytical Details

Transformation Products, Statistics, and Kinetics

Reference Substance and Reference

Substance Results

Oxidation of 1,3-butadiene with three strains of methane-utilising bacteria (Methylosinus trichosporium, methylococcus capsulantus, and methylobacterium organophilum.; Bacteria was grown in a 50% methane/50% air atmosphere and incubated in a 50% 1,3-butadiene/50% oxygen atmosphere at 30C.; Not Reported

Not Reported; Not Reported 1,2-epoxybutene; Not Reported; Not Reported

Not Reported; Not Reported

Not Reported; Not Reported

		I	EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subs	tance			
	Metric 1:	Test Substance Identity	High	The test substance was identified definitively
	Metric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 2: Test Desig	gn			
	Metric 3:	Study Controls	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 4:	Test Substance Stability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 3: Test Cond	litions			
	Metric 5:	Test Method Suitability	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 6:	Testing Conditions	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 7:	Testing Consistency	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 8:	System Type and Design	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 4: Test Orga	nisms			
Č	Metric 9:	Outcome Assessment Methodology	High	The test organism was reported; more details may be in the source cited.
	Metric 10:	Sampling Methods	N/A	This metric does not apply to this study type.

Continued on next page ...

Study Citation: OECD Harmonized	ECB, (2002). Euro	opean Union risk assessment report: 1,3	-butadiene.	
Template:	Wilsechaneous			
HERO ID:	5155560			
			EVALUATION	
Domain		Metric	Rating	Comments
	Metric 11:	Test Substance Identity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 12:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 6: Confoundin	g/Variable Control Metric 13: Metric 14:	Confounding Variables Health Outcomes Unrelated to Exposure	Medium N/A	Details regarding this metric were not reported; more details may be in the source cited. This metric does not apply to this study type.
Domain 7: Data Presen	tation and Analysis			
	Metric 15:	Data Reporting	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric does not apply to this study type

Overall Quality Determination

Metric 17:

Metric 18:

Medium

Medium

N/A

Details regarding this metric were not reported; more details may be in the source cited.

This metric does not apply to this study type.

Verification or Plausibility of

Results QSAR Models

^{*} Related References: Cited secondary source Hou et al (1979) [HERO ID 5349195]

Study Citation:	Zhao, Z., Husainy, S., Smith, G. D. (2011). Kinetics studies of the gas-phase reactions of NO3 radicals with series of 1-alkenes, dienes, cycloalkenes,
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alkenols, and alkenals. Journal of Physical Chemistry A 115(44):12161-12172.

OECD Harmonized Template:

Miscellaneous

HERO ID: 901429

	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline	None; Experimental; Experimental
Solvent, Reactivity, Storage, Stability	Nitrogen carrier gas; NR; NR; NR
Radiolabel, Source, State, Purity	NA; TCI America; Gas; 99%
Test Method Details, Test Condition Details, and	Disappearance of test material and reference substance in gas-phase reaction with NO3 measured to determine rate; Atmospheric-pressure. Reac-
Test Consistency	tion times of 6.0 - 24 seconds; Test groups used the same method. NO3 concentrations 3E10 - 2E12 molecules/cm^3
Details System Type Design	Test metarial reference commound and NO comics are in a class flow tube with flow sets of 2.0 standard literatures may be allowed to recent with NO
System Type Design	Test material, reference compound, and N2 carrier gas in a glass flow tube with flow rate of 2.0 standard liters per min allowed to react with N2 carrying N2O5 (thermally dissociates to NO3) at a flow rate of 70 standard cubic centimeters per min
Sampling Frequency and Sampling Details	Not reported; Flow leaves the flow tube and to a 523 K 1/4" o.d., 4" long vaporizer tube (to minimize condensation), to sampling ion tube region
	of a stainless steel orifice 0.5 mm i.d.
Test Temperature	$295 \pm 2 \text{ K}$
Results Details	Rate of disappearance of the gas-phase test material via NO3 + test material -> products
Analytical Method and Analytical Details	Chemical ionization method with mass spectrometer; Ions generated by 210Po source, detected using Channeltron electron multiplier
Transformation Products, Statistics, and Kinetics	Not applicable; ± 0.15 and ± 0.07 E-13 cm ³ /molecule sec; Rate of disappearance KOC: 1.23 and 1.26 E-13 cm ³ /molecule sec Plot of ln
	(OC/[OC]0) vs $ln([R]/[R]0)$ analyzed by linear least-squares fitting to obtain KOC / Kr ratio Where OC = test material; r = reference material
Reference Substance and Reference	trans-2-butene; cyclopentene; trans 2-butene KOC / Kr = 0.310 ± 0.038 cyclopentene KOC / Kr = 0.262 ± 0.012 Where Kr = rate of disappearance
Substance Results	of the reference substance

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 1: Test Substanc	e			
	Metric 1:	Test Substance Identity	High	The test substance was definitively identified.
	Metric 2:	Test Substance Purity	High	The source and purity of the test substance was reported.
Domain 2: Test Design				
	Metric 3:	Study Controls	N/A	The metric is not applicable to this study type.
	Metric 4:	Test Substance Stability	High	The test substance preparation was reported and appropriate for the study.
Domain 3: Test Condition	ns			
	Metric 5:	Test Method Suitability	High	Test method was suitable for the test substance.
	Metric 6:	Testing Conditions	High	Test conditions were monitored and reported.
	Metric 7:	Testing Consistency	High	Test conditions were consistent across study groups.
	Metric 8:	System Type and Design	N/A	The metric is not applicable to this study type.

Continued on next page ...

Study Citation:	Zhao, Z., Husainy, S., Smith, G. D. (2011). Kinetics studies of the gas-phase reactions of NO3 radicals with series of 1-alkenes, dienes, cycloalkenes,
	alkenols, and alkenals, Journal of Physical Chemistry A 115(44):12161-12172

OECD Harmonized Template:

Miscellaneous

P	
HERO ID:	901429

			EVALUATIO	V
Domain		Metric	Rating	Comments
Domain 4: Test Organisms				
M	etric 9:	Outcome Assessment Methodology	N/A	The metric is not applicable to this study type.
M	etric 10:	Sampling Methods	N/A	The metric is not applicable to this study type.
Domain 5: Outcome Assessi	nent			
M	etric 11:	Test Substance Identity	High	The outcome assessment methodology addressed the intended outcomes of interest.
М	etric 12:	Test Substance Purity	High	Sampling methods addressed the outcomes of interest, used widely acceptable methods, and no notable uncertainties were expected to influence results.
Domain 6: Confounding/Var	iable Control			
M	etric 13:	Confounding Variables	High	Sources of variability and uncertainty in the measurements and statistical techniques between study groups were considered and accounted for in data evaluation.
M	etric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
D : 7 D : D : :	1 4 1 '	•		
Domain 7: Data Presentation	-		*** 1	
М	etric 15:	Data Reporting	High	Analytical methods were suitable for detection and quantification of the target chemical and sufficient evidence was presented to confirm the parent compound disappearance was not due to other processes.
M	etric 16:	Statistical Methods and Kinetic Calculations	High	Statistical and kinetic calculations were described and appropriate for the datasets.
Domain 8: Other				
M	etric 17:	Verification or Plausibility of	High	The results were reasonable.
M	etric 18:	Results QSAR Models	N/A	The metric is not applicable to this study type.
Overall Quality 1	 Dotormin	otion	High	

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

Term	Definition
BAF	Biaccumulation Factor
BCF	Bioconcentration Factor
BMF	Biomagnification Factor
BSAF	Biota-sediment Accumulation Factor
С	Concentration
CASRN	Chemical Abstract Service registry number
DOC	Dissolved Organic Carbon
dw	Dry weight
DW	Drinking Water
DWTP	Drinking Water Treatment Plant
EPA	Environmental Protection Agency
ESI	Electrospray Ionisation
FID	Flame Ionisation Detector
FPD	Flame Photometric Detector
GC	Gas Chromatography
g/L	Grams per Liter
HLC	Henry's Law Constant
HPLC	High-performance liquid chromatography
ISO	International Organization for Standardization
Koa	Octanol-Air partition coefficient
Koc	Organic carbon-water partition coefficient
K_{ow}	Octanol-Water partition coefficient
L/d	Liters per day
LOD	Limit of Detection
LOQ	Limit of Quantification
lw	Lipid weight
M	Molarity (mol/L = moles per Liter)
mL/min	Milliliters per minute
mM	Millimolar
MDL	Method Detection Limit
mg/kg	Milligrams per Kilogram
mg/L	Milligrams per Liter
mg/m ³	Milligrams per cubic meter
MRL	Method Reporting Limit
MS	Mass Spectrometry
n	Sample Size
N/A	Not applicable
ND	Non-Detection
ng/L	Nanograms per Liter

Continued on next page ... Page 109 of 110

Term	Definition
nm	Nanometers
NR	Not Reported
OECD	Organisation for Economic Co-operation and Development
· OH	Hydroxyl radical
OPE	Organophosphate Ester
pg/L	Picograms per Liter
ppm	parts per million
QSAR	Quantatative Structure Activity Relationship
RSD	Relative Standard Deviation
SI	Supplemental Information
SIM	Selected Ion Monitoring
SPE	Solid Phase Extraction
STP	Sewage Treatment Plant
TMF	Trophic Magnification Factor
TOC	Total Organic Carbon
TOF	Time of Flight
μ g/L or μ g/mL	micrograms per liter or per milliliter
UPLC	Ultra-performance liquid chromatography
US or USA	United States of America
UV (UV-Vis)	Ultra Violet (Visible)
ww	Wet Weight
WWTP	Wastewater Treatment Plant