



Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport for 1,3-Butadiene

Systematic Review Support Document for the Draft Risk Evaluation

CASRN: 106-99-0

November 2024

PUBLIC RELEASE DRAFT November 2024

This supplemental file contains information regarding the data extraction and evaluation results for data sources that were considered for the *Draft 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 *Draft 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.

1,3-Butadiene Table of Contents

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HERO ID	Reference	Page
Photolysis in Air		
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.	5
7348613	EC, (2002). Summary risk assessment report for 1,3-butadiene.	7
5155560	ECB, (2002). European Union risk assessment report: 1,3-butadiene.	11
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.	35
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.	37
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.	39
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.	44
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.	46
660158	Klamt, A. (1993). Estimation of gas-phase hydroxyl radical rate constants of organic compounds from molecular orbital calculations. Chemosphere 26(7):1273-1289.	48
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.	50
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.	52
5589165	Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 1,3-butadiene.	54
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.	66
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.	69
3454	U.S. EPA, (1989). Health and environmental effects document for 1,3-butadiene.	73
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.	77
Hydrolysis		
6628926	NCBI, (2020). PubChem database: compound summary: 1,3-butadiene.	80

Photolysis in Water

PUBLIC RELEASE DRAFT November 2024

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: 82 1,3-butadiene. :380-381. 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: 84 1.3-butadiene. :380-381. 6628926 92 NCBI, (2020). PubChem database: compound summary: 1,3-butadiene. **Biodegradation in Sediment Biodegredation in Soil** 11779754 Howard, P. H., Boethling, R. S., Jarvis, W. F., Meylan, W. M., Michalenko, E. M. (1991). Handbook of environmental degradation rates: 96 1,3-butadiene. :380-381. **Aquatic Bioconcentration Terrestrial Bioconcentration Adsorption and Desorption** Miscellaneous 5155560 ECB, (2002). European Union risk assessment report: 1,3-butadiene. 98 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, 104 cycloalkenes, alkenols, and alkenals. Journal of Physical Chemistry A 115(44):12161-12172. **Other Properties**

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

1,3-Butadiene Photolysis in Air HERO ID: 5675250 Table: 1 of 1

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.

OECD Harmonized Template:

Details

Photolysis in Air

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-	not reported; not reported; not reported
tails	
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	not reported; not reported; not reported
by Loss Lower and Upper	
Indirect Type Results, Indirect Rate	NO3 radical rate constant (cm3/molecule sec); rate constant k dependent on k2/k-2 (K2); k = 5.6±0.8x10^-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); $k = 7.0 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 2.2x10^-11 cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 1.87 \tau 10^{-14} cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 1.87 \tau 10^{-14} cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 1.87 \tau 10^{-14} cm3/molecule); $k = 1.87 \times 10^{-14}$ (K2 value at 298K = 1.87 \tau 10^{-14} cm3/molecule); $k = 1.87 \times 10^{-14}$ (V2 value at 298K = 1.87 \tau 10^{-14} cm3/molecule); $k = 1.87 \times 10^{-14}$ (V2 value at 298K = 1.87 \tau 10^{-14} cm3/molecule); $k = 1.87 \times 10^{-14}$ (V2 value at 298K = 1.87 \times 10^{-14} (V2 value at 298K = 1.87 \tau 10^{-14} cm3/molecule); $k = 1.87 \times 10^{-14}$ (V2 value at 298K = 1.87 \tau 10^{-14} cm3/molecule); $k = 1.87 \times 10^{-14}$ (V2 value at 298K = 1.87 \tau 10^{-14} cm3/molecule); $k = 1.87 \times 10^{-14}$
Method Details Results and Products	= 7.9x10^-14 (K2 at 298K = 3.35x10^-11 cm3/molecule)
Details Results	IR spectra recorded using FTIR spectrometer; not reported
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 Degrada-	not reported; not reported; indicated error reported = two standard deviations
tion Results and Standard	
Deviation Results	
Results Remarks, Sample time Results, 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.		
	Metric 2:	Test Substance Purity	Low	The source and purity were not reported.		
Domain 2: Test Design						
	Metric 3:	Study Controls	Low	Controls were not included.		
Continued on next page						

1,3-Butadiene Photolysis in Air

... continued from previous page

HERO ID: 5675250 Table: 1 of 1

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:

5675250

onditions were not
formation may be
come of interest.

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

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	N. t. Danasta d. N. t. Danasta 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	Not Reported; Not Reported				
by Loss Lower and Upper					
Indirect Type Results, Indirect Rate	Reaction with Ozone; half-life = 1.9 days; Not Reported; Not Reported				
Constant Lower and Upper	N.D. A.I.W.D. A.I.				
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	N. t. Danasta da N. t. Danasta da N. t. Danasta d				
Results Remarks, Sample time Results, Results Details	Not Reported; 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.		
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		

HERO ID: 7348613 Table: 1 of 2

1,3-Butadiene Photolysis in Air

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

Photolysis in Air

	EVALUATION				
Domain		Metric	Rating	Comments	
	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.	
	Metric 8:	System Type and Design	N/A	Estimated value from secondary source with no citation.	
Domain 4: Test Organ			37/4		
	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	Low	No methodology was reported; no citation.	
	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to the study.	
Domain 6: Confound	ing/Variable Control	·			
Domain o. Comound	Metric 13:	Confounding Variables	N/A	Estimated value from secondary source with no citation.	
	Metric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.	
	Medic 11.	Exposure	14/11	This metric does not apply to ans study type.	
Domain 7: Data Prese	•	D (D)	т.		
	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	
	M-4 10.	Results	NT/A	possible.	
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.	
Overall Qual	lity Determin	ation	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)

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

OECD Harmonized

onized Photolysis in Air

Template:

DX/DD		TANT
EXTR	ACI	ION

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; 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 Degradation Results and Standard	Not Reported; Not Reported; Not Reported
Deviation Results Results Remarks, Sample time Results, Results 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.		
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.		

HERO ID: 7348613 Table: 2 of 2

1,3-Butadiene Photolysis in Air

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Study Citation: OECD Harmonized Template:

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

DECD Harmonized Photolysis in Air

Template: HERO ID:

7348613

	EVALUATION					
Domain		Metric	Rating	Comments		
	Metric 8:	System Type and Design	N/A	Estimated value from secondary source with no citation.		
Domain 4: Test Organ	isms					
C	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 A	Assessment					
	Metric 11:	Test Substance Identity	Low	No methodology was reported; no citation.		
_	Metric 12:	Test Substance Purity	N/A	The metric is not applicable to the study.		
Domain 6: Confoundi	ng/Variable Control					
	Metric 13:	Confounding Variables	N/A	Estimated value from secondary source with no citation.		
	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	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:	QSAR Models	N/A	A QSAR model was not reported.		

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

Photolysis in Air

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	NR; NR		
Source Wavelength Lower and Upper Test Details and Control	NR; NR		
	NR NR; NR		
Initial Concentration, Reference Compound	INK INK, INK		
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	Second order rate constant for reaction with off radicals, x=0.002 fr cm 5/molecule sec, fix		
Method Details Results and Products	NR; NR		
Details Results	ND ND		
Parameter Value and Parameter Results	NR; NR		
Reference Substance Results, Percent Degrada- tion Results and Standard	NR; NR		
Deviation Results			
Results Remarks, Sample time Results, Results	NR; NR; NR		
Details			

		EVALUATION	
	Metric	Rating	Comments
e			
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.
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.
	Metric 2: Metric 3:	Metric 1: Test Substance Identity Metric 2: Test Substance Purity Metric 3: Study Controls	Metric 1: Test Substance Identity High Metric 2: Test Substance Purity Medium Metric 3: Study Controls Medium

Continued on next page ...

1,3-Butadiene HERO ID: 5155560 Table: 1 of 12

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

Template:

HERO ID: 5155560

Photolysis in Air

]	EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Condi	tions			
	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 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.

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

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

OECD Harmonized

Photolysis in Air

Template:

EXTR	ACT	LIUI	V

	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	NID NID
Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference	NR NR; NR
Compound	AND AND
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 ozone; k=6.1E-18 cm ³ /molecule*sec; NR
Constant Lower and Upper	ND, ND
Method Details Results and Products Details Results	NR; NR
Parameter Value and Parameter Results	1.9 days; Half-life for reaction with atmospheric ozone
Reference Substance Results, Percent Degrada-	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 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	gn			
	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	

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HERO ID: 5155560 Table: 2 of 12

Study Citation: OECD Harmonized **Template:**

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

Photolysis in Air

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	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	ing/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 Preso	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 Klopffer et al. 1988 [HERO ID 1939717]

Study Citation: ECB, (2002). European Union risk assessment report: 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; 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 by Loss Lower and Upper	NR; Not Reported; NR			
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; NR			
tion Results and Standard				
Deviation Results Results Remarks, Sample time Results, Results	NR; NR; NR			
Details	THE, THE			

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subst	tance			
	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	9			
	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	litions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
			Continued on next page	

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HERO ID: 5155560 Table: 3 of 12

Study Citation: OECD Harmonized **Template:**

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

Photolysis in Air

HERO ID:

5155560

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

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

Template:

HERO ID: 5155560

EXTRACTION

	EATRACTION
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; 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	ND ND
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	0.5, 1.0, 2.0 ppm; NR
Compound	
Substance Wavelength Lower and Upper	NR; NR
D' (O (WILLD II D' (HICL'C	ND ND ND

NR; NR; NR

NR; NR

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

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

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 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				
	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	tions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
			Continued on next page	

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HERO ID: 5155560 Table: 4 of 12

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

d Photolysis in Air

Template: HERO ID:

D: 5155560

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

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

OECD Harmonized

Photolysis in Air

Template:

EXTR	A 4		

	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; 305 K
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, 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	6 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
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	NR, lefative to il-butane (k=2.09E-12 Ciff 3) inolecules. S
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	NR; NR
Details	

		EVALUATION	
	Metric	Rating	Comments
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.
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.
ions			
Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
ı	Metric 2: Metric 3: Metric 4:	Metric 1: Test Substance Identity Metric 2: Test Substance Purity Metric 3: Study Controls Metric 4: Test Substance Stability	Metric 1: Test Substance Identity High Metric 2: Test Substance Purity Medium Metric 3: Study Controls Medium Metric 4: Test Substance Stability Medium

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HERO ID: 5155560 Table: 5 of 12

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

ized Photolysis in Air

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 Lloyd et al., 1976 [HERO ID 8541109]

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

OECD Harmonized

Photolysis in Air

Template:

EXTR	A 4		

	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; 299.5 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=6.85E-11 cm^3/molecule*sec; NR
Method Details Results and Products Details Results	NR; absolute rate method
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 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	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.		
Domain 3: Test Condi	itions					
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.		
	Continued on next page					

HERO ID: 5155560 Table: 6 of 12

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

Photolysis in Air

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 Organisms			
Metric	9: Outcome Assessment Methodolog	gy 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			
Metric	17: Verification or Plausibility of	Medium	Values seem appropriate; more details may be in the source cited.
Metric	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]

1,3-Butadiene Photolysis in Air HERO ID: 5155560 Table: 7 of 12

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

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; ~300 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; NR
Indirect Type Results, Indirect Rate	Second order rate constant for reaction with OH radicals; kOH=6.51E-11 cm ³ /molecule*sec; NR
Constant Lower and Upper	Second state valuation with contraction with contractions, note of the symptotic sec, the
Method Details Results and Products	NR; relative to ethene (k=8.45E-12 cm^3/molecule*sec
Details Results	NID NID
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				
	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	tions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
		(Continued on next page	•••

HERO ID: 5155560 Table: 7 of 12

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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	iisms			
	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 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].

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

OECD Harmonized

Photolysis in Air

Template:

EXTRACTION			
	FXTR	ΔC	LIUN

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- 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=6.16E-11 cm^3/molecule*sec; kOH=6.88E-11 cm^3/molecule*sec
Method Details Results and Products Details Results	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
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 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	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.
Domain 3: Test Condi	itions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
			Continued on next page	

HERO ID: 5155560 Table: 8 of 12

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

Overall Quality Determination

^{*} 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]

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

OECD Harmonized

Photolysis in Air

Template:

EXTRACTION			
	FXTR	ΔC	LIUN

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 Source Wavelength Lower and Upper	NR; NR
Test Details and Control	NR; NR
Initial Concentration, Reference	NR NR; NR
Compound	ND ND
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 OH radicals; kOH=6.65E-11 cm^3/molecule*sec; Not Reported
Constant Lower and Upper	
Method Details Results and Products Details Results	NR; relative to propene (k=2.68E-11 cm ³ /molecule*sec
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; 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	

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HERO ID: 5155560 Table: 9 of 12

Study Citation: OECD Harmonized Template:

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

Photolysis in Air

HERO ID:

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Overall Quality Determination

			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	nnisms			
C	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	sentation 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.

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

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

OECD Harmonized

Photolysis in Air

Template:

EXTRAC	TION
LAINAC	11011

	EATRACTION
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 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 OH radicals; kOH=6.1E-11 cm^3/molecule*sec; kOH=6.8E-11 cm^3/molecule*sec
Constant Lower and Upper	
Method Details Results and Products	NR; NR
Details Results	NID. NID
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	NR; NR; NR
Details	

			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	gn			
	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	

HERO ID: 5155560 Table: 10 of 12

... continued from previous page

Study Citation: OECD Harmonized Template:

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

Photolysis in Air

HERO ID: 5155560

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

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

OECD Harmonized

Photolysis in Air

Template:

EXTRACTION			
	FXTR	ΔC	LIUN

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 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=6.85E-11 cm^3/molecule*sec; Not Reported
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 Deviation Results	NR; 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	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.
Domain 3: Test Condi	itions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
			Continued on next page	

1,3-Butadiene Photolysis in Air

... continued from previous page

HERO ID: 5155560 Table: 11 of 12

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

Photolysis in Air

Template: HERO ID:

5155560

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

Overall Quality Determination

^{*} 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]

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

OECD Harmonized

Photolysis in Air

Template:

EXTR	AC'	TIO	N

	EATRACTION
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	
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	IVE, IVE, IVE
Deviation Results	
Results Remarks, Sample time Results, Results	NR; NR; NR
Details	

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subst	tance			
	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	litions			
	Metric 5:	Test Method Suitability	Medium	Test method not reported; ; more details may be in the source cited.
		(Continued on next page	

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HERO ID: 5155560 Table: 12 of 12

Study Citation: OECD Harmonized **Template:**

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

Photolysis in Air

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 Organis	sms			
C	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	ssessment			
	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 Presen		•		
	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]

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:

11EKO 1D. 600294	
	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 de- tails	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 Degrada- tion Results and Standard Deviation Results	not reported; 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

		EVALUATIO	N	
Domain	Metric	Rating	Comments	
Oomain 1: Test Substance				
Metric 1:	Test Substance Identity	High	The test substance was identified.	
Metric 2:	Test Substance Purity	High	The source the test substance was reported.	
Oomain 2: Test Design				
e	C. 1 C 1	37/4		
Metric 3:	Study Controls	N/A	The study did not require concurrent control groups.	

HERO ID: 860294 Table: 1 of 1

1,3-Butadiene Photolysis in Air

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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:
HERO ID:

860294

]	EVALUATIO:	N
Domain		Metric	Rating	Comments
	Metric 4:	Test Substance Stability	High	The test substance preparation conditions were reported.
Domain 3: Test Condi	tions			
	Metric 5:	Test Method Suitability	High	The test method was suitable for the test substance.
	Metric 6:	Testing Conditions	High	Testing conditions were reported.
	Metric 7:	Testing Consistency	High	Test conditions were consistent.
	Metric 8:	System Type and Design	High	The system type and design were appropriate.
Domain 4: Test Organ	isms			
	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 A	Assessment Metric 11:	Test Substance Identity	Medium	There were minor differences between the assessment methodology and the intended outcome assessment.
	Metric 12:	Test Substance Purity	High	The study reported the use of sampling methods that address the outcome of interest.
Domain 6: Confoundi	ng/Variable Control			
	Metric 13:	Confounding Variables	N/A	The metric is not applicable.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable.
Domain 7: Data Prese	ntation and Analysis			
	Metric 15:	Data Reporting	High	Data reporting was appropriate.
	Metric 16:	Statistical Methods and Kinetic Calculations	Low	Statistical analysis and kinetic calculations were not described clearly.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of Results	High	The study results were reasonable.
	Metric 18:	QSAR Models	N/A	A QSAR model was not reported.
Overall Qual	ity Determin	ation	High	

1,3-Butadiene Photolysis in Air HERO ID: 5696791 Table: 1 of 1

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:

HERO ID: 5696791

HERO ID: 5696791						
	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; Not reported					
Indirect Type Results, Indirect Rate Constant Lower and Upper Method Details Results and Products Details Results	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					
Parameter Value and Parameter Results	Not reported; Not reported					
Reference Substance Results, Percent Degrada tion Results and Standard	Not reported; Not reported					
Deviation Results Results Remarks, Sample time Results, Result Details	s cyclic isomerization of beta-hydroxyalkyl radical to alpha-hydroxyalkyl radical was evident; Not reported; Not reported					
	EVALUATION					

EVALUATION				
Domain	Metric	Rating	Comments	
Domain 1: Test Substance				
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.	

HERO ID: 5696791 Table: 1 of 1

1,3-Butadiene Photolysis in Air

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 Photolys			continu	ued from pre	vious page		
Non-standard method evaluating transformation product: UV photolysis of iodolydrins. Metric 9: System Type and Design N/A The metric is not applicable to this type of study.		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.					
Domain Metric 8: Study Controls Metric 4: Test Design Metric 4: Test Substance Stability N/A The metric is not applicable to this type of study. Metric 6: Test Method Suitability N/A The metric is not applicable to this type of study. Metric 7: Testing Conditions Metric 8: System Type and Design N/A The metric is not applicable to this type of study. Metric 9: Testing Conditions High Testing Conditions High Testing Conditions High Testing Conditions were meniored, reported, and appropriate for the method. Metric 9: System Type and Design N/A The metric is not applicable to this type of study. Metric 9: Outcome Assessment Metric 9: America is not applicable to this type of study. Metric 10: Sampling Methods N/A The metric is not applicable to this type of study. Metric 12: Test Substance Identity Low The outcome assessment methodology did not specifically address the imended outcome of interest; however, Olf 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. Metric 13: Metric 14: Health Outcomes Urrelated to N/A The metric is not applicable to this type of study. Metric 13: Metric 14: Health Outcomes Urrelated to N/A The metric is not applicable to this type of study. Metric 15: Data Presentation and Analysis Metric 16: Statistical Methods and High Methods for kinetic calculations were described. Metric 17: Verification or Plausibility of Results Metric 18: White Calculations were described. Metric 18: Werification or Plausibility of Results Metric 18: Werification or Plausibility of Results Metric 18: Metric 18: Werification or Plausibility of Results Metric 18: Metric 18: Werification or Plausibility of Results Metric 18: Metric 18: Werification or Plausibility of Results Metric 18: Metric 18: Werification or Plausibility of Results Metric 18: Metric 18: Werification or Plausibility of Results Metric 18: Metric 18: Werification or Plausibility of Results Metric 18: Metric 18: Werification or Plausibilit							
Domain Metric Rating Comments 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. Metric 5: Test Method Suitability N/A The metric is not applicable to this type of study. Metric 6: Testing Conditions High Testing conditions High 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. Metric 9: Outcome Assessment Metric 10: Sampling Methods N/A The metric is not applicable to this type of study. Metric 11: Test Substance Identity N/A The metric is not applicable to this type of study. Metric 12: Test Substance Purity N/A The metric is not applicable to this type of study. Metric 13: Active Purity N/A The metric is not applicable to this type of study. Metric 14: Test Substance Purity N/A The metric is not applicable to this type of study. Metric 14: Test Substance Purity N/A The metric is not applicable to this type of study. Metric 13: Active Purity N/A The metric is not applicable to this type of study. Metric 14: Test Substance Purity N/A The metric is not applicable to this type of study. Metric 15: Active Purity N/A The metric is not applicable to this type of study. Metric 16: Substance Purity N/A The metric is not applicable to this type of study. Metric 16: Substance Purity N/A The metric is not applicable to this type of study. Metric 16: Substance Purity N/A The metric is not applicable to this type of study. Metric 16: Substance Purity N/A The metric is not applicable to this type of study. Metric 16: Substance Purity N/A The metric is not applicable to this type of study. Metric 16: Substance Purity N/A The metric is not applicable to this type of study. Metric 16: Substance Purity N/A The metric is not applicable to this type of study. Metric	Template:						
Metric 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. 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. Metric 10: Sampling Methods 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. 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. Metric 12: Test Substance Purity N/A The metric is not applicable to this type of study. The metric is not applicable to this type of study. The metric is not applicable to this type of study. Metric 13:	HERO ID:	5696791					
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Metric 18: QSAR Models High Model calculations were described.	ľ	Metric 17:	-	Low	Reported values were reasonable; however, not specific to the target chemical.		
verall Quality Determination Low	1	Metric 18:	Results QSAR Models	High	Model calculations were described.		
verall Quality Determination Low	011 0 114	D-4	49	T .			
	Overall Quality	Determin	iauon	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.

OECD Harmonized Template:

:380-381. Photolysis in Air

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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; 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	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			

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 Desi	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.

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OECD Harmonized :380-381. Photolysis in Air

Template: HERO ID:

11779754

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 Cond	litions			
	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	nisms			
- 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				
	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	ling/Variable Control			
Domain o. Comounc	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 Prac	entation and Analysis			
Domain 7. Data Pies	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.
D : 0 01				·
Domain 8: Other	3.6 . 1.7	W.C. C. DI. T.T. C.	т	
	Metric 17:	Verification or Plausibility of Results	Low	Due to limited information, evaluation of the reasonableness of the study results was n possible.
	Metric 18:	QSAR Models	N/A	This metric does not apply to this study type.

1,3-Butadiene Photolysis in Air HERO ID: 11779754 Table: 1 of 2

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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

11779754

HERO ID:	11779754			
		EVALUATION		
Domain	Metric	Rating	Comments	
Overall Qu	ality 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

OECD Harmonized Template:

HERO ID: 11779754

	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	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	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 at 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.

1,3-Butadiene Photolysis in Air HERO ID: 11779754 Table: 2 of 2

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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:

]	EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Cond	litions			
	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	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	ling/Variable Control			
Domain of Company	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	entation and Analysis			
Domain (1 Dam 110)	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	ation	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:

	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 details	OH radicals were generated by the KrF excimer laser photolysis of H2O2; Not Reported; Not Reported				
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 Compound	9.0-26 10E16 molecule/cm3; Ethene				
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 Method Details Results and Products	branching ratio (cm3/molecule sec); 6.66E-11 x 0.866 x 0.75 Rate coefficient x branching ratio (cm3/molecule sec)				
Details Results	Quantitative absorption-time profiles were simulated using the FACSIMILE program and modeling of peroxy radicals via their permutation reactions 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 Details	Not Reported; Not Reported; Not Reported				
Details					

			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	Medium	Qualitative control results were reported.
			Continued on next page	

HERO ID: 1696190 Table: 1 of 1

1,3-Butadiene Photolysis in Air

... continued from previous 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

Overall Quality Determination

HERO ID: 1696190

			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	litions			
	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 Orga	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	ling/Variable Control			
Domain or Comoune	Metric 13:	Confounding Variables	N/A	The metric is not applicable to this study.
	Metric 14:	Health Outcomes Unrelated to	N/A	The metric is not applicable to this study.
		Exposure		
Domain 7: Data Pres	entation and Analysis			
	Metric 15:	Data Reporting	Low	Analytical details were omitted.
	Metric 16:	Statistical Methods and	N/A	The metric is not applicable to the study.
		Kinetic Calculations		
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.

Uninformative

1,3-Butadiene Photolysis in Air HERO ID: 5618698 Table: 1 of 1

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

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	15 ppm 70 ppm; 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 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 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	Substance			
	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.

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HERO ID: 5618698 Table: 1 of 1

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

Metric 5: Test Method Suitability Medium Some details were omitted regarding testing conditions; however, this was not likely 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. High This metric met the criteria for high confidence as expected for this type of study. This metric met the criteria for high confidence as expected for this type of study. Domain 4: Test Organisms Metric 9: Outcome Assessment Methodology M/A The metric is not applicable to this study type. Metric 10: Sampling Methods Domain 5: Outcome Assessment Metric 11: Test Substance Identity Medium Details regarding sampling methods were not fully reported; however, the omission were not likely to have a substantial impact on results. Domain 6: Confounding/Variable Control Metric 13: Confounding Variables N/A No confounding variables were noted. Metric 14: Health Outcomes Unrelated to Exposure Domain 7: Data Presentation and Analysis Metric 15: Data Reporting Medium Some experimental data and half-life data was not reported. Medium The kinetic calculations were not described in detail but are assumed to be adequat Kinetic Calculations.	HERO ID.	3010070			
Domain 3: Test Conditions Metric 5: Test Method Suitability Medium Medium Metric 6: Testing Conditions Medium Metric 7: Testing Consistency High This metric met the criteria for high confidence as expected for this type of study. This metric met the criteria for high confidence as expected for this type of study. This metric met the criteria for high confidence as expected for this type of study. This metric met the criteria for high confidence as expected for this type of study. Domain 4: Test Organisms 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 Assessment Metric 11: Test Substance Identity Medium Medium Details regarding sampling methods were not fully reported; however, the omission were not likely to have a substantial impact on results. Domain 6: Confounding/Variable Control Metric 13: Confounding Variables Health Outcomes Unrelated to Exposure Domain 7: Data Presentation and Analysis Metric 15: Data Reporting Medium Some experimental data and half-life data was not reported. Medium The kinetic calculations were not described in detail but are assumed to be adequated to Kinetic Calculations Medium The kinetic calculations were not described in detail but are assumed to be adequated to Results					N
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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 Organisms Metric 9: Outcome Assessment Methodology M/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 Assessment 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 omission were not likely to have a substantial impact on results. Domain 6: Confounding/Variable Control Metric 13: Confounding Variables N/A No confounding variables were noted. Metric 14: Health Outcomes Unrelated to Exposure Domain 7: Data Presentation 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 adequat Kinetic Calculations Domain 8: Other Metric 17: Verification or Plausibility of High The study results were reasonable. Results		Metric 6:	Testing Conditions	Medium	Some details were omitted regarding testing conditions; however, this was not likely to have influenced the interpretation of the results.
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Metric 9: Outcome Assessment Methodology Metric 10: Sampling Methods N/A The metric is not applicable to this study type. Domain 5: Outcome Assessment Metric 11: Test Substance Identity High Medium Details regarding sampling methods were not fully reported; however, the omission were not likely to have a substantial impact on results. Domain 6: Confounding/Variable Control Metric 13: Confounding Variables N/A No confounding variables were noted. Metric 14: Health Outcomes Unrelated to Exposure Domain 7: Data Presentation and Analysis Metric 15: Data Reporting Medium Some experimental data and half-life data was not reported. Medium The kinetic calculations were not described in detail but are assumed to be adequat Kinetic Calculations Domain 8: Other Metric 17: Verification or Plausibility of Results Metric 17: Verification or Plausibility of Results		Metric 8:	System Type and Design	High	This metric met the criteria for high confidence as expected for this type of study.
Metric 9: Outcome Assessment Methodology Metric 10: Sampling Methods N/A The metric is not applicable to this study type. Domain 5: Outcome Assessment Metric 11: Test Substance Identity High Medium Details regarding sampling methods were not fully reported; however, the omission were not likely to have a substantial impact on results. Domain 6: Confounding/Variable Control Metric 13: Confounding Variables Metric 14: Health Outcomes Unrelated to Exposure Domain 7: Data Presentation and Analysis Metric 15: Data Reporting Medium Some experimental data and half-life data was not reported. Metric 16: Statistical Methods and Kinetic Calculations Metric 17: Verification or Plausibility of Results Metric 17: Verification or Plausibility of Results Metric 18: Algebra The metric is not applicable to this study type. The metric is not applicable to this study type. Some experimental data and half-life data was not reported. The kinetic calculations were not described in detail but are assumed to be adequated to the study results were reasonable. Metric 17: Verification or Plausibility of Results	Domain 4: Test Organ	nisms			
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Metric 11: Test Substance Identity Metric 12: Test Substance Purity Medium Details regarding sampling methods were not fully reported; however, the omission were not likely to have a substantial impact on results. Domain 6: Confounding/Variable Control Metric 13: Confounding Variables Metric 14: Health Outcomes Unrelated to Exposure Domain 7: Data Presentation and Analysis Metric 15: Data Reporting Metric 16: Statistical Methods and Kinetic Calculations Medium Medium Medium The outcome assessment methodology addressed the outcomes of interest. Medium Some of interest. Medium Medium The metric is not applicable to this study type. Some experimental data and half-life data was not reported. Medium Medium The kinetic calculations were not described in detail but are assumed to be adequated to the study results were reasonable. Medium The study results were reasonable.					
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were not likely to have a substantial impact on results. Domain 6: Confounding/Variable Control Metric 13: Confounding Variables Metric 14: Health Outcomes Unrelated to Exposure Domain 7: Data Presentation and Analysis Metric 15: Data Reporting Medium Metric 16: Statistical Methods and Kinetic Calculations Medium Medium The kinetic calculations were not described in detail but are assumed to be adequat Kinetic Calculations Domain 8: Other Metric 17: Verification or Plausibility of Results Medium The study results were reasonable. Results				C	e.
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Metric 13: Confounding Variables N/A No confounding variables were noted. Metric 14: Health Outcomes Unrelated to Exposure Domain 7: Data Presentation and Analysis Metric 15: Data Reporting Medium Some experimental data and half-life data was not reported. Metric 16: Statistical Methods and Kinetic Calculations Domain 8: Other Metric 17: Verification or Plausibility of Results Metric 19: Verification or Plausibility of Results Metric 19: N/A No confounding variables were noted. N/A No confounding variables were noted. N/A The metric is not applicable to this study type. Medium Some experimental data and half-life data was not reported. Medium The kinetic calculations were not described in detail but are assumed to be adequated to the indication of the properties of	Domain 6: Confound	ing/Variable Control			
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Domain 7: Data Presentation and Analysis Metric 15: Data Reporting Medium Some experimental data and half-life data was not reported. Medium The kinetic calculations were not described in detail but are assumed to be adequat Kinetic Calculations Domain 8: Other Metric 17: Verification or Plausibility of Results Medium The kinetic calculations were not described in detail but are assumed to be adequat Figure 17: Werification or Plausibility of Figure 17: Werification or Plausibility of Figure 18: Note 18: Note 19: N		Metric 14:	9	N/A	
Metric 15: Data Reporting Medium Some experimental data and half-life data was not reported. Metric 16: Statistical Methods and Kinetic Calculations Domain 8: Other Metric 17: Verification or Plausibility of Results Medium The kinetic calculations were not described in detail but are assumed to be adequated to be			Exposure		
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Metric 16: Statistical Methods and Kinetic Calculations Domain 8: Other Metric 17: Verification or Plausibility of Results Medium The kinetic calculations were not described in detail but are assumed to be adequated to		•	Data Reporting	Medium	Some experimental data and half-life data was not reported.
Domain 8: Other Metric 17: Verification or Plausibility of High The study results were reasonable. Results		Metric 16:		Medium	The kinetic calculations were not described in detail but are assumed to be adequate.
Metric 17: Verification or Plausibility of High The study results were reasonable. Results			Kinetic Calculations		
Results	Domain 8: Other				
		Metric 17:		High	The study results were reasonable.
		Metric 18:		N/A	The metric is not applicable to this study type.
Overall Quality Determination High	Overall One	lity Dotormin	otion	High	

1,3-Butadiene Photolysis in Air HERO ID: 660158 Table: 1 of 1

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

Photolysis in Air

Template:

HERO ID: 660158

EXTR	AC	ΓΙΟΝ	

	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	Not reported; Not reported
by Loss Lower and Upper	
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

Method Details Results and Products	Rate constant for OH radical addition to olefinic carbon-carbon double bonds (sp2-carbon atoms); Not reporte
Details Results	Not asserted. But a contest with 10F 12 and 2 and 1 and 4
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	
Deviation Results	

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

Metric Test Substance Identity Test Substance Purity	Rating High N/A	Comments The test substance was definitively identified. The metric is not applicable to this study type.	
<u>-</u>		· · · · · · · · · · · · · · · · · · ·	
<u>-</u>		· · · · · · · · · · · · · · · · · · ·	
Test Substance Purity	N/A	The matric is not applicable to this study type	
	11/11	The metric is not applicable to this study type.	
Study Controls	N/A	The metric is not applicable to this study type.	
Test Substance Stability	N/A	The metric is not applicable to this study type.	
	· · · · · · · · · · · · · · · · · · ·	•	

HERO ID: 660158 Table: 1 of 1

1,3-Butadiene Photolysis in Air

... continued from previous page

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

OECD Harmonized
Template:

26(7):1273-1289. Photolysis in Air

Template: HERO ID:

660158

			EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 3: Test Condit	ions			
	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.
Domain 4: Test Organi	sms			
	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 A	ssessment			
	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: Confoundin	ng/Variable Control			
	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 Presen	ntation 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				
	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.

HERO ID: 598253 Table: 1 of 1 1,3-Butadiene Photolysis in Air

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. Photolysis in Air

OECD Harmonized

Template:

HERO ID: 598253

FXTR	ACTION

	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 hydroxy radicals and ozone in the presence of nitrogen oxides
Solvent, Reactivity, Storage, Stability	NR; NR; NR
Radiolabel, Source, State, Purity	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 Degrada- tion Results and Standard Deviation Results	Not reported; Not reported
Results Remarks, Sample time Results, Results Details	Not reported; Not reported; Indoor experiments of OH-initiated photodegradation resulted in the same outcome.

EVALUATION				
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 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.

1,3-Butadiene Photolysis in Air

... continued from previous page

HERO ID: 598253 Table: 1 of 1

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

OECD Harmonized Template:

33(18):3005-3022. Photolysis in Air

HERO ID:

598253

			CTA T TARRES	A.
Domain		Metric	EVALUATIO Rating	Comments
Domain	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	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 Organ	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.
Domain 5: Outcome A			_	
	Metric 11:	Test Substance Identity	Low	Quantitative data not reported for photodegradation rates or formation of transformation products.
	Metric 12:	Test Substance Purity	High	This metric met the criteria for high confidence as expected for this type of study.
Domain 6: Confoundi	ng/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 Prese	entation 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 Qual	ity Determin	ation	Low	

1,3-Butadiene Photolysis in Air HERO ID: 3254900 Table: 1 of 1

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:

-	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 details	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 $7\pm1\%$, HCOCl $3\pm1\%$, 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- tion Results and Standard Deviation Results	Not reported; Not reported
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	Domain 1: Test Substance				
	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 Desig	gn				
	Metric 3:	Study Controls	Low	No controls were reported.	
	Continued on next page				

1,3-Butadiene Photolysis in Air

... continued from previous page

HERO ID: 3254900 Table: 1 of 1

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:

Template: HERO ID:	3254900			
		H	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.
	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 Organ	nisms			
Č	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	Assessment			
	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: Confound	ing/Variable Control			
	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 Prese	entation and Analysis			
	Metric 15:	Data Reporting	Low	Limited detail regarding analytical method; percent recovery or mass balance were no reported.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	The metric is not applicable to this study.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Low	Quantitative rate results were not reported; however, transformation products were reported.
	Metric 18:	Results QSAR Models	N/A	The metric is not applicable to this study type.
Overall Qua			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		
tails	N. D. J. I. N. D. J. I.		
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	9.0 ppb; Not Reported		
Compound	N.D. J.N.D. J.		
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		
Constant Lower and Upper			
Method Details Results and Products	Not Reported; Not Reported		
Details Results 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		

			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	Medium	The test substance source and purity were not reported.
Domain 2: Test Desig	n			
	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

HERO ID: 5589165 Table: 1 of 6

1,3-Butadiene Photolysis in Air

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

zed Photolysis in Air

Template: HERO ID:

5589165

	E	EVALUATION	
	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.
nisms			
	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
Metric 10:		N/A	Rating of this factor is not applicable to this kind of information.
	1 0		5 · · · · · · · · · · · · · · · · · · ·
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
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	N/A	Rating of this factor is not applicable to this kind of information.
	Exposure		
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	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
	Kinetic Calculations		
Metric 17:	Verification or Plausibility of	Medium	The results are reasonable based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.
Metric 18:		N/A	Rating of this factor is not applicable to this kind of information.
	Metric 6: Metric 7: Metric 8: Metric 9: Metric 10: Assessment Metric 11: Metric 12: Ing/Variable Control Metric 13: Metric 14: entation and Analysis Metric 15: Metric 16:	Metric 5: Test Method Suitability Metric 6: Testing Conditions Metric 7: Testing Consistency Metric 8: System Type and Design Misms Metric 9: Outcome Assessment Methodology Metric 10: Sampling Methods Assessment Metric 11: Test Substance Identity Metric 12: Test Substance Purity Metric 13: Confounding Variables Metric 14: Health Outcomes Unrelated to Exposure entation and Analysis Metric 15: Data Reporting Metric 16: Statistical Methods and Kinetic Calculations Metric 17: Verification or Plausibility of Results	Metric 5: Test Method Suitability Medium Metric 6: Testing Conditions Medium Metric 7: Testing Consistency Medium Metric 8: System Type and Design N/A misms Metric 9: Outcome Assessment Methodology N/A Metric 10: Sampling Methods N/A Assessment Metric 11: Test Substance Identity Medium Metric 12: Test Substance Purity Medium Metric 13: Confounding Variables Medium Metric 14: Health Outcomes Unrelated to Exposure Entation and Analysis Metric 15: Data Reporting Medium Metric 16: Statistical Methods and Kinetic Calculations Metric 17: Verification or Plausibility of Medium Results

Overall Quality Determination

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]

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; 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; 79°F		
Light Source, Intensity, and additional light de-	not reported; not reported; not reported		
tails Source Wavelength Lower and Upper	not noncettod, not noncettod		
	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	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 noncettod, not noncettod		
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-	not reported; not reported; not reported		
tion Results and Standard			
Deviation Results Results Remarks, Sample time Results, Results	not reported; not reported		
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; 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

1,3-Butadiene Photolysis in Air

... continued from previous page

HERO ID: 5589165 Table: 2 of 6

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

		I	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	Medium	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, "Hydrocarbon Reactivities in the Atmospheric Photooxidation of Nitric Oxide",. Env. Sci.Technol. 4 (11), 916-24 (1970b). [HERO ID 14872]

EXTRACTION

Study Citation:

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

0.44x10^-3/ppm min; Rate constant for NO thermal oxidation

Not Reported; Not Reported; Not Reported

OECD Harmonized

Photolysis in Air

Template:

Details Results

Details

tion Results and Standard Deviation Results

Parameter Value and Parameter Results

Reference Substance Results, Percent Degrada-

Results Remarks, Sample time Results, Results

HERO ID: 5589165

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
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; Not Reported
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported
Method Details Results and Products	Not Reported; Not Reported

EVALUATION				
	Metric	Rating	Comments	
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 in this secondary source.	
	0.10.1	N. 1.		
	•		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 no reported in the secondary source.	
ions				
Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.	
	Metric 2: Metric 3: Metric 4:	Metric 1: Test Substance Identity Metric 2: Test Substance Purity Metric 3: Study Controls Metric 4: Test Substance Stability	Metric 1: Test Substance Identity High Metric 2: Test Substance Purity Medium Metric 3: Study Controls Medium Metric 4: Test Substance Stability Medium	

Acrolein and formaldehyde were identified as NO-butadiene reaction products.; Not Reported; Not Reported

HERO ID: 5589165 Table: 3 of 6

1,3-Butadiene Photolysis in Air

... continued from previous 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

Template: HERO ID:

5589165

Overall Quality Determination

			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	nnisms			
	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 3. 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: 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 Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Pres	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 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 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).

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:

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; Not Reported	
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; Not Reported	
Indirect Type Results, Indirect Rate Constant Lower and Upper	Not Reported; Not Reported; Not Reported	
Method Details Results and Products Details Results	Rate of decrease of NO2 concentrations in the butadiene-air mixture was measured; Not Reported	
Parameter Value and Parameter Results	0.4x10^-4/ppm min; Rate constant for NO2-butadiene reaction	
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	

EVALUATION				
Domain		Metric	Rating	Comments
Domain 1: Test Substan	ice			
	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 Condition	ons			
	Metric 5:	Test Method Suitability	Medium	Test method details were not reported in the secondary source.
		C	ontinued on next page	

1,3-Butadiene Photolysis in Air

... continued from previous page

HERO ID: 5589165 Table: 4 of 6

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

DECD Harmonized Photolysis in Air

Template: 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 Organi	isms			
Č	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 A	ssessment			
	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: Confoundin	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/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:

Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 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; experimental; other: not specified	
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	24 hr; 40-45°F	
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	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	2.4 ppb; 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; Not Reported	
Constant Lower and Upper	not reported, not reported	
Method Details Results and Products	Not Reported; Not Reported	
Details Results		
Parameter Value and Parameter Results	0 ppb; Concentration of butadiene after 24 hr UV Irradiation	
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		

		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	

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HERO ID: 5589165 Table: 5 of 6

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

armonized Photolysis in Air

Template: HERO ID:

5589165

Me Me Domain 4: Test Organisms Me Me Domain 5: Outcome Assessm Me	etric 6: etric 7: etric 8: etric 9: etric 10: etric 11:	Metric Testing Conditions Testing Consistency System Type and Design Outcome Assessment Methodology Sampling Methods Test Substance Identity	EVALUATION Rating Medium Medium N/A N/A N/A	Comments 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. 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. Rating of this factor is not applicable to this kind of information. Rating of this factor is not applicable to this kind of information. Rating of this factor is not applicable to this kind of information.
Me Me Domain 4: Test Organisms Me Me Domain 5: Outcome Assessm Me	etric 7: etric 8: etric 9: etric 10:	Testing Consistency System Type and Design Outcome Assessment Methodology Sampling Methods	Medium N/A N/A	inclusion in a peer-reviewed/recognized database or other secondary source. 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. Rating of this factor is not applicable to this kind of information. Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organisms Me Me Domain 5: Outcome Assessm Me	etric 8: etric 9: etric 10:	System Type and Design Outcome Assessment Methodology Sampling Methods	N/A	clusion in a peer-reviewed/recognized database or other secondary source. Rating of this factor is not applicable to this kind of information. Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organisms Me Me Domain 5: Outcome Assessm Me	etric 9: etric 10:	Outcome Assessment Methodology Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Me Me Domain 5: Outcome Assessm Me	etric 10:	Sampling Methods		
Me Me Domain 5: Outcome Assessm Me	etric 10:	Sampling Methods		•
Domain 5: Outcome Assessm Me	nent		N/A	Rating of this factor is not applicable to this kind of information.
Me		Test Substance Identity		
	etric 11:	Test Substance Identity		
		200 2 assume rating	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.
Me	etric 12:	Test Substance Purity	Medium	Sampling methodology is unknown is unknown but is likely to be appropriate based or the data's inclusion in a peer-reviewed/recognized database or other secondary source.
Domain 6: Confounding/Varia	able Control			
Me	etric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
Me	etric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Presentation	and Analysis			
	etric 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.
Me	etric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
Me	etric 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.
Me	etric 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]

Study Citation:

Parsons, T. B., Wilkins, G. E. (1976). Biological effects and environmental aspects of 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; experimental; other: not specified	
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	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. Starting concentration: 2.8 ppb; after 24 hr in dark; 2.6 ppb	
Initial Concentration, Reference	2.6 ppb; 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	
Constant Lower and Upper		
Method Details Results and Products	Not Reported; Not Reported	
Details Results Parameter Value and Parameter Results	0 ppb; Concentration of butadiene after 24 hr UV Irradiation	
Reference Substance Results, Percent Degrada-	Not Reported; Not Reported	
tion Results and Standard	The Reported, The Reported	
Deviation Results		
Results Remarks, Sample time Results, Results	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.	
Domain 2: Test Design Metric 3:	Study Controls	Medium		
	Study Controls		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		

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HERO ID: 5589165 Table: 6 of 6

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

Photolysis in Air

Template: HERO ID:

5589165

			EVALUATION	
Domain		Metric	Rating	Comments
M	letric 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.
M	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.
N	letric 8:	System Type and Design	N/A	Rating of this factor is not applicable to this kind of information.
Domain 4: Test Organisms				
N	letric 9:	Outcome Assessment Methodology	N/A	Rating of this factor is not applicable to this kind of information.
N	Metric 10:	Sampling Methods	N/A	Rating of this factor is not applicable to this kind of information.
Domain 5: Outcome Assess	sment			
M	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.
M	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: Confounding/Va	riable Control			
N	letric 13:	Confounding Variables	Medium	Sources of variability and uncertainty were not reported in the secondary source.
M	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	Rating of this factor is not applicable to this kind of information.
Domain 7: Data Presentatio	n 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.
M	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	No statistical methods or kinetic calculations were reported in the secondary source.
Domain 8: Other				
M	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.
M	letric 18:	QSAR Models	N/A	Rating of this factor is not applicable to this kind of information.
Overall Quality			Medium	Taking of the factor is not approved to the line 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

Template:

Photolysis in Air

HERO ID: 618974

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 details	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 Compound	1.513, 1.996, 1.120 ppm; Not applicable		
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 Degradation Results and Standard	Not applicable; Not applicable		
Deviation Results 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		

		EVALUATIO:	N
Domain	Metric	Rating	Comments
Domain 1: Test Substance			
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

1,3-Butadiene Photolysis in Air

... continued from previous page

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.

HERO ID: 618974 Table: 1 of 1

OECD Harmonized

Template:

Photolysis in Air

			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 Condi	tions			
	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 Organ	isms			
	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 A	Assessment Metric 11: Metric 12:	Test Substance Identity Test Substance Purity	High High	The outcome assessment methodology addressed or reported the intended outcome of interest. 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: Confoundi	ng/Variable Control			
	Metric 13:	Confounding Variables	N/A	No confounding variables were noted.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
Domain 7: Data Prese	ntation 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				
	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.
		Conti	nued on next p	page

HERO ID: 618974 Table: 1 of 1

1,3-Butadiene Photolysis in Air

4.	•	•	
continued	from	previous	nage

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

HERO ID: 618974

		EVALUATION	
Domain	Metric	Rating	Comments

Overall Quality Determination

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; NR
Radiolabel, Source, State, Purity	NA; Aldrich Chemical Co.; NR; >/= 99.0%
Duration and Test Temperature	$2-7 \min; 298 \pm 2 \text{ K}$
Light Source, Intensity, and additional light de- tails	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	Not Reported; NR; NR
by Loss Lower and Upper	
Indirect Type Results, Indirect Rate	OH radical (in the presence of NO); NR; NR
Constant Lower and Upper	5500 T. G L
Method Details Results and Products	7500 L Teflon chamber at ~5% relative humidity, samples analyzed by GC-FID; Acrolein (0.55 ű 0.05), HCHO (0.62 ű 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-	Not Reported; 53%; NR

			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	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

tion Results and Standard Deviation Results

Details

HERO ID: 1742345 Table: 1 of 2

1,3-Butadiene Photolysis in Air

... continued from previous page

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

Template:

Photolysis in Air

			EVALUATION	
Domain		Metric	Rating	Comments
	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.
	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 Organ	nisms			
	Metric 9:	Outcome Assessment Methodology	N/A	Not applicable.
	Metric 10:	Sampling Methods	N/A	Not applicable.
Domain 5: Outcome	Assessment			
2 smain 3. Gutcome	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: Confound	ing/Variable Control			
	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 Prese	entation and Analysis			
	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	Low	The results deviated significantly from previously reported product yields.
	Metric 18:	Results QSAR Models	N/A	Not applicable.
Overall Oua	lity Determin	ation	Medium	

1,3-Butadiene Photolysis in Air HERO ID: 1742345 Table: 2 of 2

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

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

OECD Harmonized

Template:

Details

Photolysis in Air

	EATRACTION
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; $298 \pm 2 \text{ K}$
Light Source, Intensity, and additional light de-	Two parallel banks of black lamps; NR; 20% maximum light intensity used; NR
tails	000 NP
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	Not Reported; NR; NR
by Loss Lower and Upper	
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 ± 0.15), and R(ONO2)(OONO2) species (0.08 – 0.16)
Parameter Value and Parameter Results	Not Reported; Not Reported
Reference Substance Results, Percent Degrada-	Not Reported; NR; NR
tion Results and Standard	
Deviation Results	
Results Remarks, Sample time Results, Results	Not Reported; NR; 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.

HERO ID: 1742345 Table: 2 of 2

1,3-Butadiene Photolysis in Air

... continued from previous page

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

Template:

	17 123 13			
			EVALUATION	
Domain		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.
Oomain 4: Test Organ	nisms			
	Metric 9:	Outcome Assessment Methodology	N/A	Not applicable.
	Metric 10:	Sampling Methods	N/A	Not applicable.
Domain 5: Outcome A	Assessment			
	Metric 11:	Test Substance Identity	Medium	The outcome assessment methodology was appropriate for determining overall loss are
	M 4 : 10	T (C) (D)	TT' 1	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: Confoundi	ng/Variable Control			
Domain o. Comound	Metric 13:	Confounding Variables	High	Uncertainty in measurements and variability were explicitly addressed through approp
	Wietric 13.	Comounting variables	High	ate statistical methods.
	Metric 14:	Health Outcomes Unrelated to	N/A	Not applicable.
		Exposure		••
Domain 7: Data Prese	ntation and Analysis			
	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	N/A	Statistical and kinetic calculations were not conducted.
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Low	The results deviated significantly from previously reported product yields for most pro-
		Results		ucts except organic nitrates.
	Metric 18:	QSAR Models	N/A	Not applicable.

1,3-Butadiene Photolysis in Air HERO ID: 3454 Table: 1 of 2

Study Citation: U.S. EPA, (1989). Health and environmental effects document 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	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	Not Reported Not Reported; Not Reported			
Compound	N. P. L. I. N. P. L. I.			
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; Not Reported			
Constant Lower and Upper	Not Reported, Not Reported			
Method Details Results and Products	Not Reported; Not Reported			
Details Results				
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; Degradation product from reaction with ozone: Acrolein			
Details	Two reported, Two reported, Degradation product from reaction with ozone. Actolem			

			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.
			Continued on next p	page

1,3-Butadiene Photolysis in Air HERO ID: 3454 Table: 1 of 2

... continued from previous page

Study Citation:
OECD Harmonized
Template:
TTER O TR

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

onized Photolysis in Air

Template:	Thotorysis in 7th				
HERO ID:	3454				
			EVALUATIO	N	
Domain		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 Organi	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.	
Domain 5: Outcome A	ssessment				
	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			
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.	
Overall Quali	tv Determins	ation ——	High		

1,3-Butadiene Photolysis in Air HERO ID: 3454 Table: 2 of 2

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

OECD Harmonized

Photolysis in Air

Template: HERO ID:

HERO ID: 3454	
	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; Not Reported
Duration and Test Temperature	Not Reported; 25 deg C
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	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; 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	Not Reported; Not Reported
Reference Substance Results, Percent Degrada- tion Results and Standard Deviation Results	Not Reported; Not Reported; Not Reported
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	ce			
	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 Condition	ons			
	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 p	page

1,3-Butadiene Photolysis in Air HERO ID: 3454 Table: 2 of 2

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Study Citation:

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

OECD Harmonized	Photolysis in Air			
Геmplate:				
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 Organis	ms			
	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 As	sessment			
	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: Confounding	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 Present	ation and Analysis			
	Metric 15:	Data Reporting	N/A	This metric is not applicable to this study type.
	Metric 16:	Statistical Methods and Kinetic Calculations	N/A	This metric is not applicable to this study type.
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 Quali	ty Determina	ation	High	

1,3-Butadiene Photolysis in Air HERO ID: 5699949 Table: 1 of 1

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

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	EXTRACTION			
Parameter	Data			
CACDN and Track Massacial	Not Demostrack 1.2 Destractions			
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	100 contentuation maged from 110 to 110 ft of 100 ft of 100 ft			
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	bimolecular rate constant k^II OH + 1,3-Butadiene (10 $^{-11}$ cm3 molecule-1 s-1); 3.15 \pm 0.28 (at 423K); 8.57 \pm 0.42 (at 263K)			
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^II) 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- tion Results and Standard	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-1); OH + 1,3-butadiene-d6 at 300K (1,3-butadiene-d6: 2.2-14.24x10^11 cm-3) k^II = 6.94 ± 0.38 x10^-11 cm3 molecule-1			
Deviation Results	s-1 (value based on 15 experiments); not reported; reported with values: \pm uncertainties represent 2 standard deviations			
Results Remarks, Sample time Results, Results Details	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 = $7.68\pm0.30x10^{-11}$ 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 = $6.96\pm0.68x10^{-11}$ 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 = $7.01\pm0.45x10^{-11}$ 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 = $6.99\pm0.28x10^{-11}$ cm3 molecule-1 s-1 (value based on 54 experiments)			
	EXALUATION			

EVALUATION

... continued from previous page

HERO ID: 5699949 Table: 1 of 1

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

OECD Harmonized

and Theses Doctoral Dissertation:213. Photolysis in Air

Template:

Template: HERO ID:	5699949			
		I	EVALUATIO	N
Domain		Metric	Rating	Comments
Domain		Metric	Rating	Comments
Domain 1: Test Subst	ance			
	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 Desig	n			
	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	itions			
	Metric 5:	Test Method Suitability	High	The test method was suitable.
	Metric 6:	Testing Conditions	High	Testing conditions were monitored, reported, and appropriate for the method.
	Metric 7:	Testing Consistency	Medium	Variable [He], [1,3-butadiene], and number of experiments run at several temperatures.
	Metric 8:	System Type and Design	High	The system type and design were appropriate.
Domain 4: Test Organ	nieme			
Domain 4. Test Organ	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. This metric is not applicable to the study type.
	1120110 101	Samping Hemods	1,111	The medic is not approache to the study type.
Domain 5: Outcome A				
	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: Confoundi	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 Prese	entation and Analysis			
	Metric 15:	Data Reporting	High	Data reporting was appropriate.
	Metric 16:	Statistical Methods and	High	Kinetic calculations were described and address the data.
		Kinetic Calculations		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	High	The study results were reasonable and compared to previously reported literature values
	Metric 18:	Results QSAR Models	N/A	This metric is not applicable to the study type.

1,3-Butadiene Photolysis in Air HERO ID: 5699949 Table: 1 of 1

... continued from previous page

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

OECD Harmonized and Theses Doctoral Dissertation:213. Photolysis in Air

Template:

		EVALUATION		
Domain	Metric	Rating	Comments	
Overall Quality Dete	ermination	High		

1,3-Butadiene Hydrolysis HERO ID: 6628926 Table: 1 of 1

Study Citation:

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

OECD Harmonized

Hydrolysis

Template:

HERO ID: 6628926

Parameter De	Data Control of the C
CASRN and Test Material 10	06-99-0; 1,3-Butadiene
Confidentiality, Type, Guideline no	ione; not specified; Not Reported: not specified
Solvent, Reactivity, Storage, Stability NI	NR; NR; NR
Radiolabel, Source, State, Purity NI	NR; NR; NR Notes: NR
Buffer, Test Temperature, Number of Replicates NI	NR; NR
Positive Controls and Negative Controls Po	Positive: NR; Negative: NR
pH and Duration NI	NR; NR
Sampling Frequency and Test Setup NI	NR; NR
Concentration No.	Not Reported
Analytical Method, Analytical Details, and NI	NR; NR; NR
Statistics Transformation Products NI	JID.
Reference Substance and Reference NI Substance Results	NR; NR
	NR; NR; NR
Constant, and Half-life	
Results Remarks No	Not expected to undergo hydrolysis in the environment due to a lack of hydrolyzable functional groups

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substar	nce			
	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 Design				
	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 Condit	ions			
	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.

1,3-Butadiene Hydrolysis HERO ID: 6628926 Table: 1 of 1

... continued from previous page

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

Hydrolysis

HERO ID:

6628926

Overall Quality Determination

			EVALUATION	
Domain		Metric	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 Asse	essment			
	Metric 11:	Test Substance Identity	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/V	Variable Control			
C	Metric 13:	Confounding Variables	Medium	Details regarding this metric were not reported in this secondary source.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to the study.
Domain 7: Data Presentat	ion and Analysis			
	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		
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	Low	Results were limited to a qualitative assessment.
	Metric 18:	Results QSAR Models	N/A	The metric is not applicable to the study.

Medium

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

1,3-Butadiene Photolysis in Water HERO ID: 11779754 Table: 1 of 1

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

EXTR	AC'	Γ	N

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; 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 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				
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 Substar	nce			
	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				
	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.

1,3-Butadiene Photolysis in Water HERO ID: 11779754 Table: 1 of 1

... continued from previous 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 in Water

Template: HERO ID:

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 3: Test Cond				
	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	nisms			
Domain II Test orga	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.
		1 0		The second secon
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	ling/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.
Damain 7, Data Bross	antation and Analysis			
Domain 7: Data Pres	entation and Analysis Metric 15:	Data Reporting	Medium	Data reporting was limited, the analytical method was not reported; however, the infor-
	Wietite 13.	Data Reporting	Wicdiani	mation is presented in a trusted secondary source.
	Metric 16:	Statistical Methods and	Medium	Kinetic and calculation details were not reported; however, the information is presented
		Kinetic Calculations		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	

^{*} 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

Template:

HERO ID: 11779754

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; 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; 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	Ground water half-life: 336 hours (14 days) - 1344 hours (8 weeks); scientific judgement based on estimated aqueous aerobic biodegradation half-lives.; NR				
Results Mean Total Recovery and Results per Recovery	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	N/A	This metric is not applicable to the data type.	
D 2. T4 D: -	_				
Domain 2: Test Desig			-		
	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.	

Biodegradation in Water 1,3-Butadiene HERO ID: 11779754 Table: 1 of 4

... continued from previous 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:

EVALUATION						
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	Testing conditions were not reported and citations were not provided.		
	Metric 7:	Testing Consistency	N/A	This metric is not applicable to the data type.		
	Metric 8:	System Type and Design	N/A	This metric is not applicable to the data type.		
Domain 4: Test Organ	isms					
Domain ii 10st organi	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	ggaggmant			***		
Domain 5. Outcome A	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	This metric is not applicable to the data type.		
Domain 6: Confoundin	•					
	Metric 13:	Confounding Variables	Low	Confounding variables were not discussed.		
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	This metric does not apply to this study type.		
		Exposure				
Domain 7: Data Preser	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: 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

	TWEN LOWYOU
	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
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	NR; NR; NR
Parameter, and 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	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

			EVALUATIO1	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.

Biodegradation in Water HERO ID: 11779754 Table: 2 of 4 1,3-Butadiene

... continued from previous 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: HERO ID:

]	EVALUATIO:	N
Domain		Metric	Rating	Comments
Domain 3: Test Cond	litions			
	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 Orga	nisms			
C	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			
Bomain 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	ling/Variable Control			
	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 Pres	entation and Analysis			
Domain 7. Data Fies	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 Qua	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.

OECD Harmonized

:380-381. Biodegradation in Water

Template:

11/19/34	
	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; 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

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Substan	ice			
	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.
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	N/A	This metric is not applicable to the data type.
Domain 3: Test Conditi	ons			
	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.
		C	Continued on next page	•••

1,3-Butadiene Biodegradation in Water HERO ID: 11779754 Table: 3 of 4

... continued from previous 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 :380-38 Biodegr

:380-381. Biodegradation in Water

Template:

HERO ID:

		•	EVALUATION	
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 Organ	nisms			
	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			
	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			
	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 Prese	entation 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 Kinetic Calculations	N/A	This metric does not apply to this study type.
Domain 8: Other				
2 cmain o. Onici	Metric 17:	Verification or Plausibility of	Low	Due to limited information, evaluation of the reasonableness of the study results was no
		Results		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.

OECD Harmonized

:380-381. Biodegradation in Water

Template:

	EXTRACTION
Parameter	Data
CASRN and Test Material	106-99-0; 1,3-butadiene
Confidentiality, EndPoint, Type,	No; Aqueous biodegradation; Calculation (scientific judgement); other: NR
Guideline Solvent, Reactivity, Storage, Stability	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	NR; NR: NR; NR
Sampling Frequency pH Adjusted and pH	NR; NR
Concentration	NR NR - NR NR NR
	NR; NR
Composition and Test Temperature	·
CEC, Water Aeration Dilution, Continuous Darkness, and Other Design	NR; NR; NR
Results Details Method, Results per Degradation	NR; NR; NR
Parameter, and	
Direct Quantum Yield Results	
Results Value, Results Standard Deviation, Re-	NR; NR; NR
sults Sample Time, and Results Reference Sub- stance Compartments	
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
covery	

		EVALUATIO1	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.

... continued from previous 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: HERO ID:

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: HERO ID:

	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; 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 Sampling Frequency	Not reported; Not Reported: Not reported
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 Dark-	Not reported; Not reported; Not reported
ness, and Other Design Results Details Method, Results per Degradation Parameter, and Direct Quantum Yield Results	Not reported; Aerobic biodegradation half-life; anaerobic biodegradation half-life; Not Reported
Results Value, Results Standard Deviation, Results Sample Time, and Results Reference Substance Compartments	7 days; 28 days; Not reported; Not reported
Results Remarks and Results Details	Not reported; Not reported
Results Mean Total Recovery and Results per Recovery	Not reported; Not reported

	EVALUATION	
Metric	Rating	Comments
Test Substance Identity	High	The test substance was identified clearly.
Test Substance Purity	Medium	Details regarding this metric were not reported in this secondary source.
Study Controls	Medium	Limited data is presented in this secondary source.
Test Substance Stability	Medium	Limited data is presented in this secondary source.
Test Method Suitability	Medium	Limited data is presented in this secondary source.
	Test Substance Identity Test Substance Purity Study Controls Test Substance Stability	Metric Rating Test Substance Identity High Test Substance Purity Medium Study Controls Medium Test Substance Stability Medium

1,3-Butadiene Biodegradation in Water HERO ID: 6628926 Table: 1 of 2

... continued from previous page

Study Citation: NCBI, (2020). PubChem database: compound summary: 1,3-butadiene. **OECD Harmonized** Biodegradation in Water **Template: HERO ID:** 6628926 **EVALUATION** Domain Metric Rating Comments Testing Conditions Metric 6: 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 Organisms Metric 9: Outcome Assessment Methodology Low Limited data is presented in this secondary source.

Domain 5: Outcome	e Assessment		
	M-4 11.	T4 C-1-4 Id4'4	

Metric 10:

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.

N/A

The metric is not applicable to this study type.

Domain 6: Confounding/Variable Control

Metric 13: Confounding Variables Medium Limited data is presented in this secondary source.

Metric 14: Health Outcomes Unrelated to Exposure

Medium Limited data is presented in this secondary source.

N/A This metric is not applicable to this type of study.

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

Domain 8: Other

Metric 17: Verification or Plausibility of 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 Quality Determination

Medium

Sampling Methods

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

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

Biodegradation in Water

Template:

EXTR	ACTION

	EXTRACTION
Parameter	Data
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	Not Donoutod, Not appointed
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 Dark-	Not reported; Not reported; Not Reported; Not reported
ness, and Other Design	
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; Not reported
sults Sample Time, and Results Reference Sub-	+ //, Not reported, Not reported
stance Compartments	
Results Remarks and Results Details	Not reported; Not reported
Results Mean Total Recovery and Results per Re-	Not reported; Not reported
covery	1, 1
•	

		EVALUATION	
Domain	Metric	Rating	Comments
Domain 1: Test Substance			
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 Conditions			
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.

1,3-Butadiene Biodegradation in Water HERO ID: 6628926 Table: 2 of 2

... continued from previous page

Study Citation: OECD Harmonized Template:

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

Biodegradation in Water

HERO ID: 6628926

		E	VALUATION	
Domain		Metric	Rating	Comments
	Metric 8:	System Type and Design	High	Reported as similar to an OECD Guideline study.
Domain 4: Test Orga	nisms			
	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: Confound	ling/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 Pres	sentation 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	Medium	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 Quality Determination

Medium

^{*} 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.

:380-381.

OECD Harmonized

Biodegredation in Soil

Template:

Parameter

HERO ID: 11779754

EXTRACTION	

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

Confidentiality, EndPoint, Type, no; other; Calculation (scientific judgement); other: NR

Data

Guideline

Solvent, Reactivity, Storage, Stability NR: NR: NR: NR

Radiolabel, Source, State, Purity NR; 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 other; NR; NR

Bulk Density

Soil Classification, Microbial Biomass, and Hu-NR; NR: NR

midity

Duration, Parameter, System, and NR; NR; NR; NR

Sampling Frequency

Control and Blank NR; NR

Concentration NR NR - NR NR NR NR: NR: NR

Analytical Method, Analytical Details, and Re-

sults Per Degredation Parameter

Results Remarks Results Value, Standard Deviation Results, Sam-

ple Time Results, Reference Substance Results, and Referencs Substance Compartment Results

Results Details Mean Total Recovery Results and Results Per Re-

covery

NID		

NR; NR; NR; NR; NR

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.
Domain 2: Test Desig	n			
	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.

Half-life: 168-672 hours (7 days-4weeks) in soil; scientific judgement based upon estimated aqueous aerobic biodegradation half-lives.

Biodegredation in Soil HERO ID: 11779754 Table: 1 of 1 1,3-Butadiene

... continued from previous 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. Biodegredation in Soil

Template: HERO ID:

]	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	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	nisms			
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 ssessment			
Bomain J. Outcome 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: Confound	ing/Variable Control			
Domain or Comound	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	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 Oug	lity Determin	ation	Low	

Study Citation:

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

OECD Harmonized

Miscellaneous

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 Test Consistency	Oxidation of 1,3-butadiene with 27 strains of propane-utilising bacteria; Bacteria was incubated in a 50% 1,3-butadiene/50% oxygen atmosphere at 30C.; Not Reported
Details 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				
Me	etric 1:	Test Substance Identity	High	The test substance was identified definitively
Me	etric 2:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited
Domain 2: Test Design				
Me	etric 3:	Study Controls	Medium	Details regarding this metric were not reported; more details may be in the source cited
Me	etric 4:	Test Substance Stability	Medium	Details regarding this metric were not reported; more details may be in the source cited
Domain 3: Test Conditions				
Me	etric 5:	Test Method Suitability	Medium	Details regarding this metric were not reported; more details may be in the source cited
Me	etric 6:	Testing Conditions	Medium	Details regarding this metric were not reported; more details may be in the source cited
Me	etric 7:	Testing Consistency	Medium	Details regarding this metric were not reported; more details may be in the source cited
Me	etric 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				
Me	etric 9:	Outcome Assessment Methodology	High	The test organism was reported; more details may be in the source cited.
Me	etric 10:	Sampling Methods	N/A	This metric does not apply to this study type.
Me	etric 10:	1 0	N/A	This metric does not apply to this study type.

1,3-Butadiene Miscellaneous

continued from previous page

HERO ID: 5155560 Table: 1 of 3

			nunuea irom previou	s page
Study Citation:	ECB, (2002). E	European 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: Confoundin	g/Variable Control	1		
Domain o. Comounain	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 Presen	tation and Analysi	is		
	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		11.7 7.71
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 Quality Determination

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].

1,3-Butadiene Miscellaneous HERO ID: 5155560 Table: 2 of 3

Study Citation:

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

OECD Harmonized

Substance Results

Miscellaneous

Template:

FYTD.	ACTION
	ACTION.

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	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
Test Consistency	volume.; Not Reported
Details 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	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			
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.

1,3-Butadiene Miscellaneous

... continued from previous page

HERO ID: 5155560 Table: 2 of 3

Study Citation: OECD Harmonized

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

Template:

			EVALUATION	
Domain		Metric	Rating	Comments
Domain 5: Outcome Assessm	nent			
Me	etric 11:	Test Substance Identity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Me	etric 12:	Test Substance Purity	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Domain 6: Confounding/Vari	able Control			
Me	etric 13:	Confounding Variables	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Me	etric 14:	Health Outcomes Unrelated to	N/A	This metric does not apply to this study type.
		Exposure		
Domain 7: Data Presentation	and Analysis	3		
Me	etric 15:	Data Reporting	Medium	Details regarding this metric were not reported; more details may be in the source cited.
Me	etric 16:	Statistical Methods and	N/A	This metric does not apply to this study type
		Kinetic Calculations		
Domain 8: Other				
Me	etric 17:	Verification or Plausibility of	Medium	Details regarding this metric were not reported; more details may be in the source cited.
	10	Results	37/4	
Me	etric 18:	QSAR Models	N/A	This metric does not apply to this study type.
Overall Quality I) Determin	nation	Medium	

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

1,3-Butadiene Miscellaneous

Study Citation:

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

OECD Harmonized

Miscellaneous

Template:

Parameter

HERO ID: 5155560

FYTD.	ACTION
	~~

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

Data

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

Test Method Details, Test Condition Details, and Ox

Test Consistency

Details

System Type Design

Sampling Frequency and Sampling Details Test Temperature

Results Details
Analytical Method and Analytical Details

Transformation Products, Statistics, and Kinetics

Reference Substance and Reference

Substance Results

0; 1,3-Butadiene
erimental; experimental

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 atmo-

HERO ID: 5155560 Table: 3 of 3

sphere at 30C.; Not Reported resting cell suspensions Not Reported; Not Reported Not Reported

Not Reported; Not Reported

Not Reported

1,2-epoxybutene; Not Reported; Not Reported

Not Reported; Not Reported

		E	VALUATION	
Domain		Metric	Rating	Comments
Domain 1: Test Subst	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 Organ	nisms			
	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.

1,3-Butadiene Miscellaneous

... continued from previous page

HERO ID: 5155560 Table: 3 of 3

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

Miscellaneous

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: Confound	ling/Variable Contro	1		
	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 Pres	entation and Analysi	is		
	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 Quality Determination

Medium

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

1,3-Butadiene Miscellaneous HERO ID: 901429 Table: 1 of 1

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

Miscellaneous

Template:

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 Test Consistency	Disappearance of test material and reference substance in gas-phase reaction with NO3 measured to determine rate; Atmospheric-pressure. Reaction times of 6.0 - 24 seconds; Test groups used the same method. NO3 concentrations 3E10 - 2E12 molecules/cm^3			
Details 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 Reference Substance and Reference Substance Results	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 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 of the reference substance			

EVALUATION				
Domain		Metric	Rating	Comments
Domain 1: Test Subst	ance			
	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 Desig	n			
	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 Condi	itions			
	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.

HERO ID: 901429 Table: 1 of 1

1,3-Butadiene Miscellaneous

... continued from previous 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

Miscellaneous

Template: HERO ID:

		H	EVALUATIO	N
Domain		Metric	Rating	Comments
Domain 4: Test Organi	sms			
	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 A	ssessment			
	Metric 11:	Test Substance Identity	High	The outcome assessment methodology addressed the intended outcomes of interest.
	Metric 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: Confoundin	ng/Variable Control			
	Metric 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.
	Metric 14:	Health Outcomes Unrelated to Exposure	N/A	The metric is not applicable to this study type.
		Exposure		
Domain 7: Data Preser	ntation and Analysis			
	Metric 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.
	Metric 16:	Statistical Methods and Kinetic Calculations	High	Statistical and kinetic calculations were described and appropriate for the datasets.
Domain 8: Other				
	Metric 17:	Verification or Plausibility of	High	The results were reasonable.
	Metric 18:	Results QSAR Models	N/A	The metric is not applicable to this study type.
Overall Quali	24 - D - 4 ! -	-49	High	

PUBLIC RELEASE DRAFT November 2024

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
C	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
Kow	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

Continued on next page ... Page 106 of 107

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

... continued from previous page

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