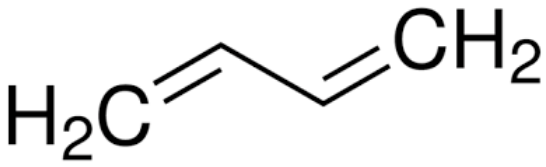
United States
Environmental Protection Agency

November 2024
Office of Chemical Safety and
Pollution Prevention

Draft Physical Chemistry, Fate, and Transport Assessment for 1,3-Butadiene

Technical Support Document for the Draft Risk Evaluation

CASRN 106-99-0



November 2024

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

ABBREVIATIONS AND ACRONYMS

atm·m3/mol	Atmospheres - cubic meters per mole
BCF	Bioconcentration factor
BAF	Bioaccumulation factor
C	Celsius
CASRN	Chemical Abstract Service registry number
cP	Centipoise
EPA	Environmental Protection Agency
g/cm^3	grams per cubic centimeter
HLC	Henry's Law constant
K_{OA}	Octanol-air partition coefficient
K_{OC}	Organic carbon-water partition coefficient
K_{OW}	Octanol-water partition coefficient
mg/L	Milligrams per liter
NIST	National Institute of Standards and Technology
NLM	National Library of Medicine
OECD	Organisation for Economic Co-operation and Development
POTW	Publicly owned treatment works
TRI	Toxics Release Inventory
TSCA	Toxic Substance Control Act
VP	Vapor pressure
WQP	Water Quality Portal
WWTP	Wastewater treatment plant
WS	Water solubility

ACKNOWLEDGEMENTS

The Assessment Team gratefully acknowledges the participation, review, and input from U.S. Environmental Protection Agency (EPA or the Agency) Office of Pollution Prevention and Toxics (OPPT) and Office of Chemical Safety and Pollution Prevention (OCSPP) senior managers and science advisors.

Docket
Supporting information can be found in the public docket, Docket ID: EPA-HQ-OPPT-2024-0425.

Disclaimer
Reference herein to any specific commercial products, process or service by trade name, trademark, manufacturer, or otherwise does not constitute or imply its endorsement, recommendation, or favoring by the United States Government.

Authors: Aderonke Adegbule, Melody Bernot, and Nicholas Blelloch

Contributors: Juan Bezares-Cruz, Marcy Card, Sheila Healy, Danielle Johnson, David Lynch, and James Sanders

Technical Support: Mark Gibson, Hillary Hollinger, Grace Kaupas, and Kelley Stanfield

This draft technical support document was reviewed and cleared for release by OPPT and OCSPP leadership.

SUMMARY

This draft technical document is in support of the Toxic Substances Control Act (TSCA) *Draft Risk Evaluation for 1,3-Butadiene*. See the draft risk evaluation for a complete list of all the technical support documents for 1,3-butadiene.

EPA considered all reasonably available information identified by the Agency through its systematic review process under TSCA (U.S. EPA, 2024h) to characterize the physical and chemical properties of 1,3-butadiene as well as the environmental fate and transport of 1,3-butadiene. The following points summarize the chemical properties and expected fate of 1,3-butadiene:

- It is a colorless gas with a mildly aromatic or gasoline-like odor. 1,3-butadiene is moderately soluble in aqueous systems (solubility = 735 mg/L).
- It is a highly volatile organic compound with a boiling point of 4.54 °C and a vapor pressure of 1900 mm Hg; 1,3-butadiene exists in gaseous phase at ambient temperatures.
- Partitioning values for 1,3-butadiene indicate low sorption to soil, sediment, or organic matter (log K_{OC} = 1.73, log K_{OW} = 1.99).
- It is expected to have limited persistence in air ($t_{1/2}$ = 1.5–9 hours), aerobic soils or sediment ($t_{1/2}$ = 7–28 days), and water ($t_{1/2}$= 1–70 hours). 1,3-Butadiene may be persistent in anaerobic media such as benthic sediments; however, it is unlikely to be found in such media ($t_{1/2}$ = 1–4 months)
- It is not likely to be persistent in the environment based on its partitioning and transformation rates. Furthermore, bioconcentration of 1,3-butadiene is expected to be low (log BCF = 0.98).
- It will photodegrade with a half-life ranging from 1.6 to 2.6 hours to form formaldehyde and acrolein when it reacts with hydroxyl radicals in the atmosphere.
- Air is expected to be the major pathway of concern for 1,3-butadiene in the environment.

1 INTRODUCTION

This draft assessment presents the physical and chemical properties of 1,3-butadiene and the environmental fate and transport of 1,3-butadiene for the draft risk evaluation conducted under the Frank R. Lautenberg Chemical Safety for the 21st Century Act, which amended TSCA on June 22, 2016.

1.1 Scope of the Risk Evaluation

The TSCA risk evaluation of 1,3-butadiene comprises several human health, environmental, fate, and exposure assessment modules, and a risk evaluation document. A diagram showing the relationships between assessments is provided in Figure 1-1. This physical chemistry and fate assessment is one of five technical support documents that are outlined in green.

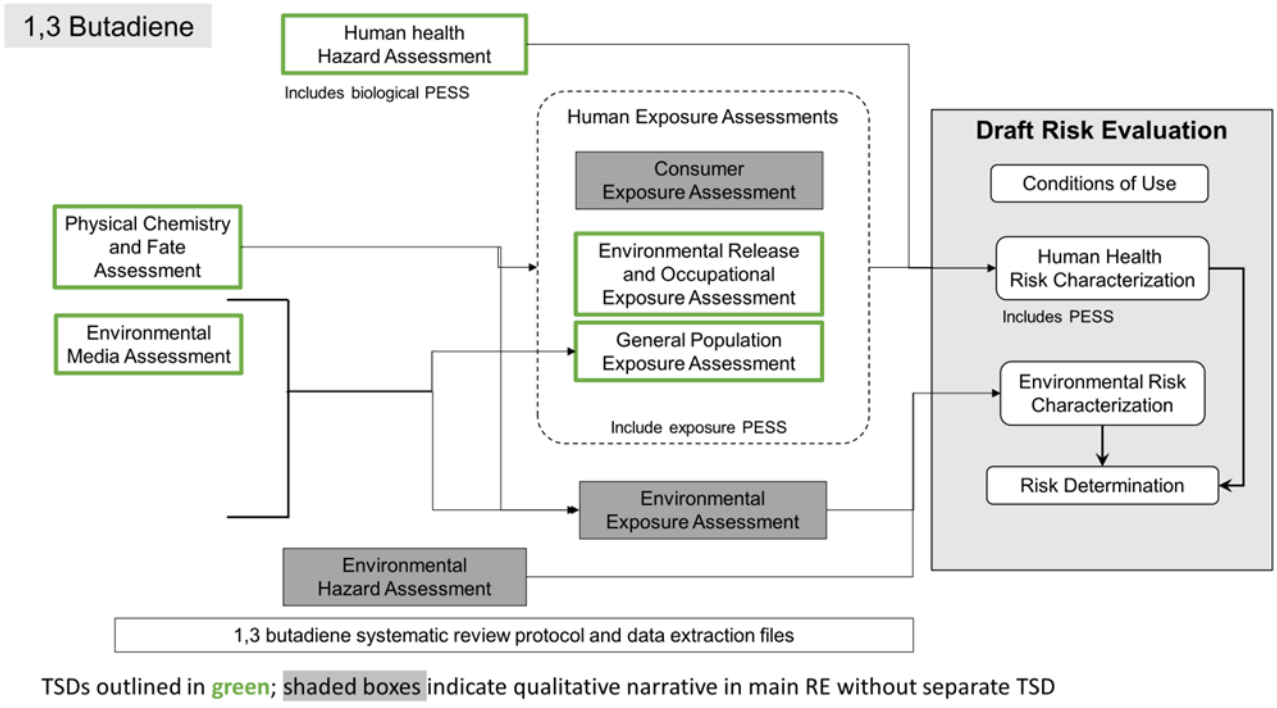


Figure 1-1. Risk Assessment Document Map Summary

1.2 Approach and Methodology

EPA gathered and evaluated physical and chemical property data and information according to the process described in the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances, Version 1.0: A Generic TSCA Systematic Review Protocol with Chemical-Specific Methodologies* (also called the "2021 Draft Systematic Review Protocol Supporting TSCA Risk Evaluations" (U.S. EPA, 2021). During the evaluation of 1,3-butadiene, EPA considered both measured and estimated physical and chemical property data (Table 2-1).

Reasonably available environmental fate data, including biotic and abiotic biodegradation rates, removal during wastewater treatment, volatilization from lakes and rivers, and organic carbon:water partition coefficient (log K_{OC}), were used to evaluate environmental fate and transport (Table 3-1). In assessing the environmental fate and transport of 1,3-butadiene, EPA considered the full range of results from sources that were rated high- and medium-quality. Details on the rating criteria are contained in the 2021 Draft Systematic Review Protocol Supporting TSCA Risk Evaluations (U.S. EPA, 2021). Information on the full extracted datasets are available in the supplemental file: *Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport Studies for 1,3-Butadiene* (U.S. EPA,

2024a) and *Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties for 1,3-Butadiene* (U.S. EPA, 2024b). Measured data were not available for the following fate properties of 1,3-butadiene: organic carbon:water partition coefficient, air:water partition coefficient, octanol:air partition coefficient, wastewater treatment efficiency and bioaccumulation factor. Thus fate estimates were based on modeling results from EPI Suite™ (U.S. EPA, 2012a), a predictive tool for physical, chemical, and environmental fate properties. EPI Suite™ was reviewed by the EPA Science Advisory Board (SAB, 2007) and the individual models that comprise EPI Suite™ have been peer reviewed through publication in technical journals. Citations for the supporting manuscripts are available in the EPI Suite help files.

1.2.1 EPI Suite™ Model Inputs and Settings

To parameterize EPI Suite™ for estimating environmental fate properties of 1,3-butadiene, the physical and chemical properties were input based on the values listed in Table 2-1. EPI Suite™ was then run using default settings. The estimated fate properties are bioconcentration factor (BCF), bioaccumulation factor (BAF), wastewater treatment plant (WWTP) removal efficiency, and partition coefficients. Figure 1-2 below is a screen shot of the EPI Suite™ interface showing the input parameters used.

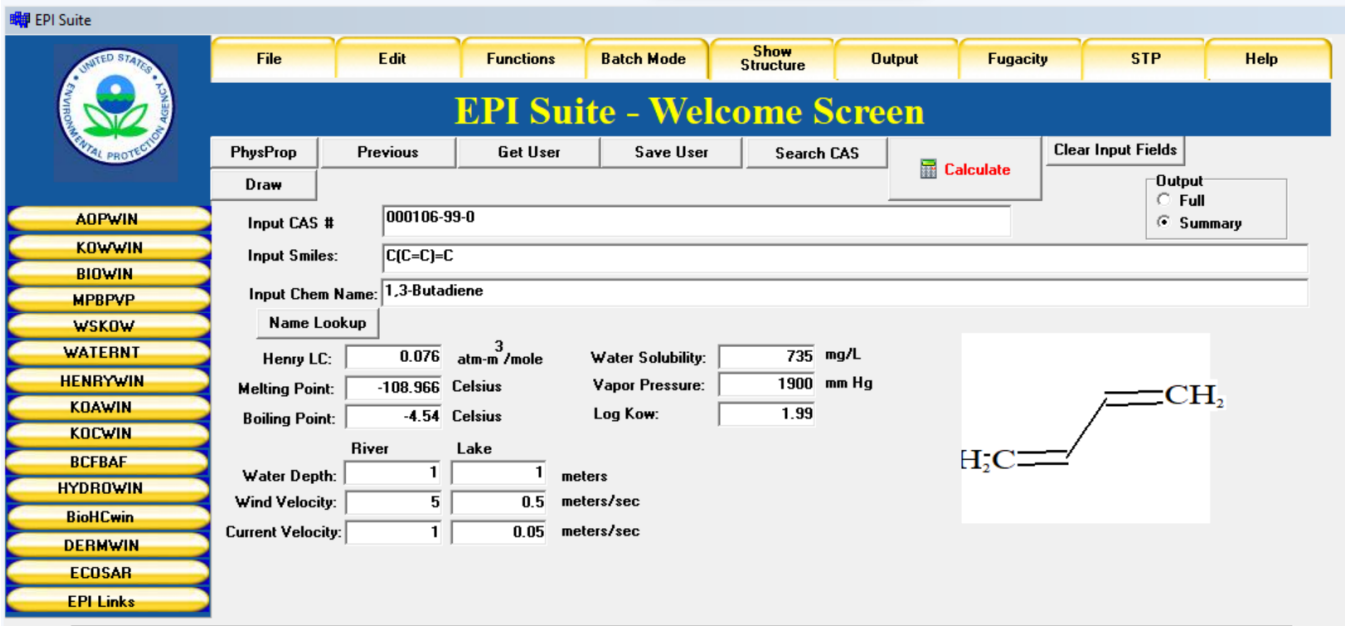


Figure 1-2. Screen Capture of EPI Suite™ Parameters Used To Calculate Fate and Physical and Chemical Properties For 1,3-Butadiene

1.2.2 Evidence Integration for Fate and Transport Properties of 1,3-Butadiene

EPA gathered and evaluated physical and chemical property data and environmental fate information according to the process described in the 2021 Draft Systematic Review Protocol Supporting TSCA Risk Evaluations (U.S. EPA, 2021). During the evaluation of 1,3-butadiene, EPA considered both measured and estimated data and information as applicable. Information and full extracted datasets are available in the supplemental file *Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport Studies for 1,3-Butadiene* (U.S. EPA, 2024a) and data evaluation information is available in the supplemental file *Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties for 1,3-Butadiene* (U.S. EPA, 2024b). The values selected are based on an overall judgement of the strength of the scientific evidence and conclusions regarding the properties and fate of 1,3-butadiene. All judgments about the strength of the evidence are based upon consideration of consistency, study design, study conditions, and uncertainty.

2 PHYSICAL AND CHEMICAL PROPERTIES OF 1,3-BUTADIENE

The systematic review process identified multiple data with high- and medium- quality ratings for many physical and chemical properties of 1,3-butadiene (U.S. EPA, 2021). Most of the data were collected under standard environmental conditions (*i.e.*, 20–25 °C and 760 mm Hg). These data are presented in Table 2-1 and box and whisker plots (Figure 2-1), which also include descriptive statistics for the dataset such as the mean and median.

Table 2-1. Physical and Chemical Properties of 1,3-Butadiene

Property	Selected Value(s)	Reference(s)	Data Quality Rating
Molecular formula	C_4H_6		
Molecular weight	54.09 g/mol		
Physical form	Colorless gas with mildly aromatic or gasoline-like odor	Rumble (2018c), NLM (2003)	High
Melting point	−109 °C	O'Neil (2013)	High
Boiling point	−4.54 °C	NIST (2022)	High
Density	0.62 g/cm^3 at 20 °C	OEHHA (2014)	High
Vapor pressure	1900 mm Hg at 20 °C	National Toxicology Program (NTP) (1993)	High
Vapor density	1.87 (air = 1)	NLM (2003)	High
Water solubility	735 mg/L at 20 °C	NLM (2003)	High
Octanol/water partition coefficient (log K_{OW})	1.99	Rumble et al. (2018)	High
Henry's Law constant	0.076 atm·m^3/mol at 25 °C	Rumble (2018a)	High
Flash point	−76.1 °C	Kerns et al. (2002)	High
Autoflammability	417.8 °C	Sun and Wristers (2002)	High
Viscosity	0.0075 cP at 20 °C (gas)	NLM (2003)	High
Refractive index	1.4292 at −25 °C	Rumble (2018c)	High

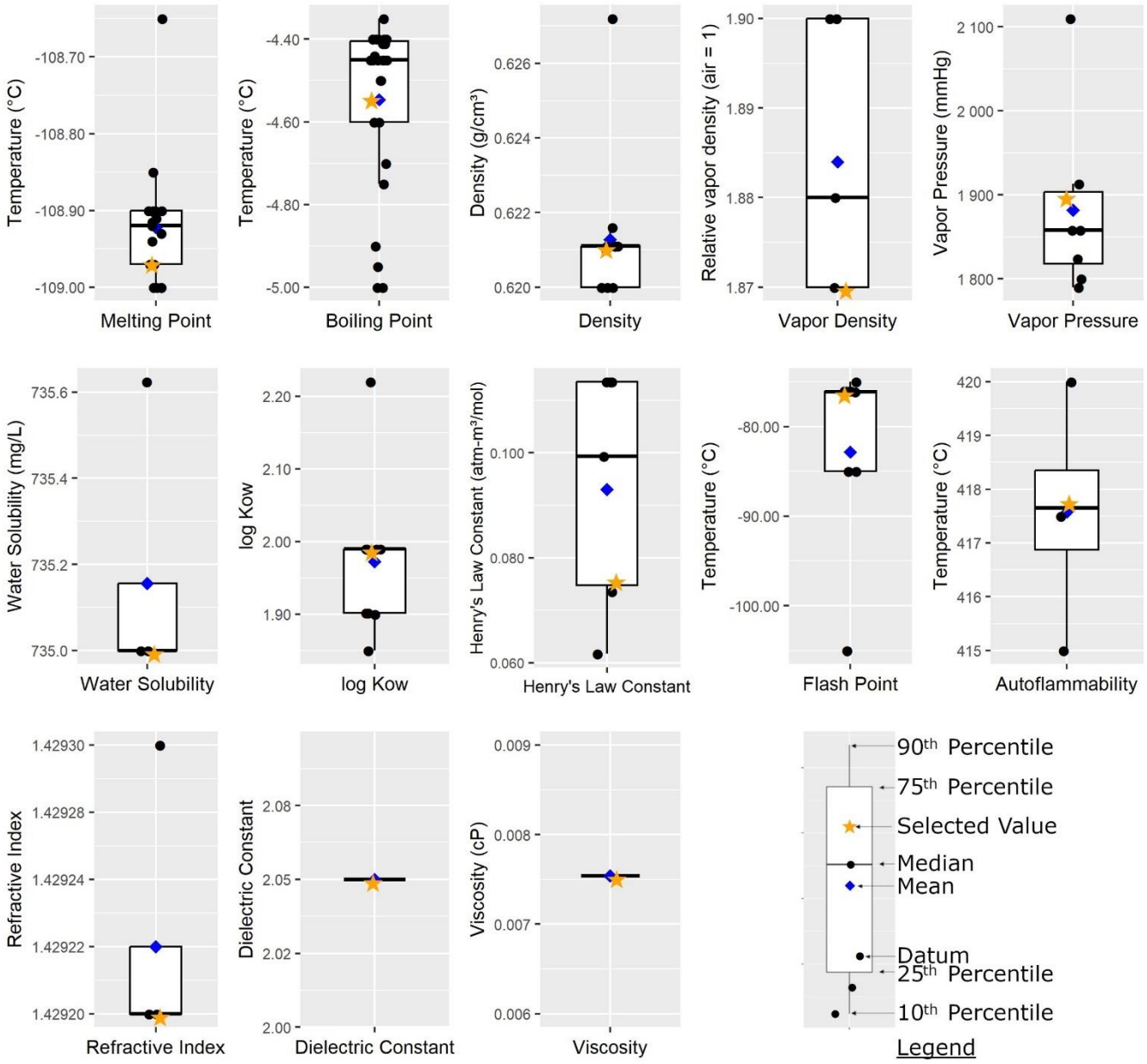


Figure 2-1. Physical-Chemical Property Data for 1,3-Butadiene under Standard Conditions
Standard conditions are 20 to 25 °C and 760 mm Hg; collected through systematic review.

To determine specific values for each parameter Table 2-1, priority was given to data from expert-curated, peer-reviewed databases that have been identified as "trusted sources" as detailed in Appendix K in the 2021 Draft Systematic Review Protocol Supporting TSCA Risk Evaluations (U.S. EPA, 2021). Where no data were available from trusted databases, second preference was given to measured data from studies that implement experimental measurements according to established test guidelines or which are conducted according to accepted standard analytical methods, including but not limited to OECD guidelines or other developed standards with sufficient documentation.

2.1 Molecular Formula and Weight

The molecular formula of 1,3-butadiene is C_4H_6. This parameter was not obtained by systematic review and there is no uncertainty in this value. The molecular weight of 1,3-butadiene is 54.09 g/mol. This

value was not obtained by systematic review, but rather was calculated from the known molecular formula. The uncertainty in this value is inherent to molecular weight determination from atomic masses and is negligible.

2.2 Physical Form

1,3-Butadiene is a gas under ambient conditions (*i.e.*, at ~20 °C and 760 mm Hg) (Rumble, 2018c). It is qualitatively described as being colorless and having an aromatic or gasoline-like odor (NLM, 2003). These descriptions agree with the qualitative descriptions identified in the *Final Scope of the Risk Evaluation for 1,3-Butadiene; CASRN 106-99-0* (also called "final scope for 1,3-butadiene") (U.S. EPA, 2020).

2.3 Melting and Boiling Point

Melting point data range from −108.966 to −108.65 °C. The average melting point of the 19 data points was −109 ± 0.08 °C. The value −109 °C from a high-quality study (O'Neil, 2013) was selected as the melting point of 1,3-butadiene for this risk evaluation and it aligns with the value reported (−108.966 °C) in the final scope for 1,3-butadiene (U.S. EPA, 2020). The standard deviation of the collected data is relatively low, indicating that the value of this parameter is well-defined (Figure 2-1).

Boiling point data collected under standard conditions ranged from −5 to −2.6 °C. Excluding statistical outliers, the range condensed to a range of −5 to −4.35 °C and averaging −4.55 ± 0.22 °C. The value −4.54 °C from a high-quality study (NIST, 2022) was selected as the boiling point of 1,3-butadiene for this risk evaluation because it is closer to the average value than the value reported (−4.5 °C) in the final scope for 1,3-butadiene (U.S. EPA, 2020). The standard deviation of the collected data (excluding outliers) is relatively low, indicating that the value of this parameter is well-defined (Figure 2-1).

2.4 Density

Density values collected at 20 °C and under standard conditions ranged from 0.62 to 0.6272 g/cm^3 (specific gravity and density were assumed to be equal). The average density of the 12 data points was 0.621 ± 0.002 g/cm^3 at 20 °C. The value 0.62 g/cm^3 at 20 °C (OEHHA, 2014) was selected as the density of 1,3-butadiene for this risk evaluation because it is closer to the average value than the value reported (0.6149 g/cm^3) in the final scope for 1,3-butadiene (U.S. EPA, 2020). The standard deviation of the collected data is relatively low, indicating that the value of this parameter is well-defined (Figure 2-1).

2.5 Vapor Density

Five vapor density data points were identified through systematic review that cover the range 1.87 to 1.9 (relative to air = 1 g/cm^3). The average of the data was 1.88 ± 0.02. The value 1.87 (NLM, 2003) was selected as the vapor density of 1,3-butadiene for this risk evaluation because it is in close agreement with the average of all the data identified, is independently reported in multiple high-quality studies, and aligns with the value reported (1.87) in the final scope for 1,3-butadiene (U.S. EPA, 2020). The standard deviation of the collected data is relatively low, indicating that the value of this parameter is well-defined (Figure 2-1).

2.6 Vapor Pressure

Vapor pressure data points included nine values collected at 20 °C. The data collected under standard conditions cover the range 910 to 2,110 mm Hg. Excluding statistical outliers, the range condensed to eight values ranging from 1,790 to 2,110 mm Hg and averaging 1,882 ± 102 mm Hg at 20 °C. The value 1,900 mm Hg at 20 °C (National Toxicology Program (NTP), 1993) from a high-quality study was

selected as the vapor pressure of 1,3-butadiene for this draft risk evaluation because it is closer to the average value than the value reported (2,110 mm Hg) in the final scope for 1,3-butadiene (U.S. EPA, 2020). The standard deviation of the collected pressure information (excluding outlier) is relatively low, indicating that the value of this parameter is well-defined (Figure 2-1).

2.7 Water Solubility

Four water solubility values were identified, all very similar at 20 °C (735–736 mg/L). The average water solubility of the four data was 735 ± 0.3 mg/L. The value 735 mg/L (NLM, 2003) was selected as the water solubility of 1,3-butadiene for this risk evaluation because it was independently reported in multiple high-quality studies, and it aligns with the value reported in the final scope for 1,3-butadiene (U.S. EPA, 2020). The standard deviation of the collected data is relatively low, indicating that the value of this parameter is well-defined (Figure 2-1).

2.8 Octanol/Water Partition Coefficient (log K_{OW})

Ten log K_{OW} data points were identified ranging from 1.84 to 2.22. The average log K_{OW} of the 10 data was 1.97 ± 0.10. The value 1.99 (Rumble et al., 2018) was selected as the log K_{OW} of 1,3-butadiene for this risk evaluation because it is in close agreement with the data identified, was independently reported in multiple high-quality studies, and aligns with the value reported in the *Final Scope of the Risk Evaluation for 1,3-Butadiene* (U.S. EPA, 2020). The standard deviation of the collected data is relatively low, indicating this parameter was well-defined (Figure 2-1).

2.9 Henry's Law Constant

Seven Henry's Law constant data points were identified through systematic review covering the range 0.062 to 0.113 atm m^3/mol. The average Henry's Law constant of the seven data was 0.093 ± 0.022 atm m^3/mol. The value 0.076 atm m^3/mol at 25 °C (Rumble, 2018a) was selected as the Henry's Law constant of 1,3-butadiene for this draft risk evaluation because it is the high-quality data point that most closely agrees with the average and it is the value referenced in the final scope for 1,3-butadiene (U.S. EPA, 2020)—although a different number (0.204 atm·m3 /mol at 25°C) was printed in error. There is considerable variance in the data collected, indicating that the value of this parameter is poorly defined (Figure 2-1).

2.10 Flash Point

Flash point values identified through systematic review range from −105 to −75 °C. Flash point data can be collected using either open cup or closed cup techniques, but many references did not indicate which technique was used. The average flash point value was −83 ± 12 °C. The value −76.1 °C (Kerns et al., 2002) was selected as the flash point of 1,3-butadiene for this risk evaluation because it is a high-quality study and aligns with the value reported in the final scope for 1,3-butadiene (U.S. EPA, 2020). Due to the multiple experimental methods for quantifying flash point (*e.g.,* open cup and closed cup), there is considerable variance in the data collected indicating that the value of this parameter is poorly defined (Figure 2-1).

2.11 Autoflammability

Four autoflammability values identified through systematic review ranged from 415 to 420 °C. The average autoflammability of the four data points was 417 ± 2 °C. The value 417.8 °C from a high-quality study (Sun and Wristers, 2002) was selected as the autoflammability of 1,3-butadiene for this draft risk evaluation because it is closer to the average value than the value reported (420 °C) in the final scope for 1,3-butadiene (U.S. EPA, 2020). The standard deviation of the collected data is relatively low, indicating that the value of this parameter is well-defined (Figure 2-1).

2.12 Viscosity

Four viscosity data points were identified through systematic review, all under different experimental conditions. The value 0.0075 cP at 20 °C was selected from a high quality study as the viscosity for gaseous 1,3-butadiene (NLM, 2003). The selected gas data was the most relevant to environmental conditions and aligns with the value reported in the final scope for 1,3-butadiene (U.S. EPA, 2020) (Figure 2-1).

2.13 Refractive Index

Twelve refractive index data points were identified through systematic review, including four data points collected at −25 °C. The data collected at −25 °C cover the range 1.4292 to 1.4293. The average refractive index of the four data points was 1.4292 ± 0.00005 at −25 °C. The value 1.4292 at −25 °C (Rumble, 2018c) was selected as the refractive index of 1,3-butadiene for this draft risk evaluation because it is in close agreement with this analysis. It is the same value reported in the final scope for 1,3-butadiene (U.S. EPA, 2020). The other eight data points were not considered because they all were at different temperatures, making it difficult to calculate an average. The standard deviation of the collected data at −25 °C is relatively low, indicating that this parameter is well-defined (Figure 2-1).

2.14 Dielectric Constant

One data point for dielectric constant was identified through systematic review from a high-quality study. The value 2.05 at 25 °C (Rumble, 2018c) was selected as the dielectric constant of 1,3-butadiene for this risk evaluation. It is the same value reported in the final scope for 1,3-butadiene (U.S. EPA, 2020) (Figure 2-1).

3 ENVIRONMENTAL FATE AND TRANSPORT OF 1,3-BUTADIENE

3.1 Final Evidence Integration for Fate and Transport Properties

Systematic review yielded relatively few available data for fate endpoints as compared to the physical and chemical property endpoints. Because of this, studies with an overall data quality determination of Medium were considered alongside those rated high for use in determining the representative fate properties of 1,3-butadiene for the purposes of the draft risk evaluation. The available studies are discussed in detail later in this section.

3.2 Final Selected Fate and Transport Property Values for 1,3-Butadiene

Table 3-1. Final Environmental Fate and Transport Characteristics of 1,3-Butadiene

Property or Endpoint	Selected Value(s) [a] [b]	Reference(s)	Data Quality Rating
Indirect photodegradation in air	$t_{1/2}$ = 1.9 h (assuming 12-hour day, 1.5E6 OH/cm^3)	Klamt (1993)	High
	$t_{1/2}$ = 1.6–2.6 hours (assuming 12-hour day, 1.5E6 OH/cm^3)	Khaled et al. (2019)	High
	$t_{1/2}$ = 1.7–1.9 hours (assuming 12-hour day, 1.5E6 OH/cm^3)	Vimal (2008)	High
	$t_{1/2}$ = 5–9 hours (assuming 5E8 NO_3/cm^3)	Andersson and Ljungström (1989)	High
	$t_{1/2}$ = 3 hours (assuming 5E8 NO_3/cm^3)	Zhao et al. (2011)	High
	$t_{1/2}$ = 34 hours [b] (assuming 7E11 O_3/cm^3)	U.S. EPA (2012b)	High
	$t_{1/2}$ = 0.76–9 hours	Howard et al. (1991)	Not Rated
Indirect photolysis in water	50–2,000 days (estimated)	Howard et al. (1991)	Not Rated
Hydrolysis	Not expected to undergo hydrolysis in the environment due to a lack of hydrolysable functional groups	NCBI (2020), Howard et al. (1991)	Not Rated
Biodegradation in water	4% aerobic biodegradation in 28 days (OECD 301D)	NCBI (2020)	Medium
	7–28 days (aerobic, estimated)	Howard et al. (1991)	Not Rated
	4–16 weeks (anaerobic, estimated)	Howard et al. (1991)	Not Rated
Biodegradation in sediment/soils	7–28 days (estimated)	Howard et al. (1991)	Not Rated
Wastewater treatment	96.6% removal (estimated)[b]	U.S. EPA (2012b)	High
Bioconcentration factor (BCF)	9.55 (estimated)[b]	U.S. EPA (2012b)	High

Property or Endpoint	Selected Value(s) [a] [b]	Reference(s)	Data Quality Rating
Organic Carbon:Water partition coefficient (log K_{OC})	1.73 (estimated)[b]	U.S. EPA (2012b)	High
Octanol:Water partition coefficient (log K_{OW})	1.99	Rumble (2018b)	High
Air:Water partition coefficient (log K_{AW})	0.49 (estimated)[b]	U.S. EPA (2012b)	High
Octanol:Air partition coefficient (log K_{OA})	1.50–1.53 (estimated)[b]	U.S. EPA (2012b)	High

[a] Measured unless otherwise noted
[b] Estimated values from EPI Suite™ physical property inputs: log K_{OW} = 1.99; BP = −4.54°C; MP = −109 °C; VP = 1,900 mm Hg; WS = 735 mg/L; HLC = 0.076 atm-m^3/mole

3.3 Partitioning

Partitioning values indicate low sorption to soil, sediment (log K_{OC} = 1.73), or organic matter in water (log K_{OW} = 1.99). A Henry's Law constant of 0.076 atm·m^3/mol at 25 °C indicates rapid volatilization from surface water and soil surfaces. Thus, with over 90 percent of releases going to air, it is expected to be the major pathway of concern for 1,3-butadiene in the environment. The biodegradation rates upon which partitioning values were derived are estimations based on scientific judgement (Howard et al., 1991). For aerobic biodegradation in water, we had two data points indicating both rapid (estimated) and slow (measured) biodegradation in water; however, the measured data was lacking experimental details so there is some uncertainty associated with it. The fugacity modeling was carried out for both fast (see Table 3-2) and slow (not shown) biodegradation and the results were similar. This is because of the volatility of 1,3-butadiene. Overall, 1,3-butadiene is primarily released to, and will generally partition to, air where it will be rapidly photodegraded (half-life = 0.76–9 hours).

3.3.1 Fugacity Modeling

EPA ran the level III fugacity model in EPI Suite™ to predict how environmental releases of 1,3-butadiene partition between environmental compartments. The model predicts the partitioning of a substance released to air, water, soil, and sediment and identifies important partitioning processes. The Level III Fugacity model is a steady-state, non-equilibrium model that includes the processes of degradation, advection (flow out of the evaluative environment) and intermedia transfer. Physical and chemical properties used as input to the model are described in Section 2 and summarized in Table 2-1. Additionally, environmental fate properties from Table 3-1 were also used as input to the model. The model was run holding the environmental release steady at a default rate of 1,000 kg/hour but varying the receiving medium (*i.e.*, air, water, soil). Releases were modeled for 1,000 kg/hour simultaneously to air, soil, and water (33% of release each) and 1000 kg/hour released only to air, soil, or water (100% of release each). Additionally, TRI releases for 2021 (99.1% of release to air, 0.1% release to land, and 0.1% release to water) were modeled (U.S. EPA, 2024f). The 0.8 percent documented as off-site releases were not included in the modeling because it was unclear to what compartment they were being released. A total of five iterations were conducted (Table 3-2).

Table 3-2. EPI Suite™ Level III Fugacity Modeling for 1,3-Butadiene Showing Partitioning for Different Media Release Scenarios[a] Assuming Constant Release

Release Scenario	Air (%)	Water (%)	Soil (%)	Sediment (%)
100% Air	99.96	0.03	0.01	<0.001
100% Water	0.89	98.7	<0.001	0.39
100% Soil	33.1	1.64	65.3	0.006
33% Air, 33% Water, 33% Soil	3.86	92.8	2.97	0.36
99.8% Air, 0.1% Water, 0.1% Soil (TRI)	94.0	5.79	0.20	0.02

[a] Modeling used half-life values of 2.6 hours in air, 28 days in water, 28 days in soil, and 16 weeks in sediment (see Table 2-1).

The fugacity modeling results suggests that if 1,3-butadiene is released solely to soil, a majority will partition to air, if released only as air emissions, 1,3-butadiene will predominantly stay in air and if released solely to water, 1,3-butadiene will predominantly stay in water (assuming constant release). Based on the reported TRI emissions contained in the *Draft Environmental Release for 1,3-Butadiene* (U.S. EPA, 2024d), only 0.1 percent of environmental releases of 1,3-butadiene are going to water. 1,3-Butadiene will primarily be released to and stay in air. Thus, the fugacity modeling from EPI Suite™ supports the classification of air as the major compartment for 1,3-butadiene.

3.4 Transformation Processes

1,3-Butadiene may undergo various transformation processes in environmental media that affect persistence and retention within the environment. Transformation processes include biodegradation, and photodegradation. Hydrolysis in environmental waters is not expected to be a significant process for 1,3-butadiene based on its lack of hydrolyzable functional groups (NCBI, 2020; Howard et al., 1991).

3.4.1 Biodegradation

Aerobic biodegradation half-life of 1,3-butadiene in water and soil is reported to be 7 to 28 days (Howard et al., 1991), though the J-check database documents results of an OECD 301D equivalent test where only 4 percent biodegradation was measured in 28 days in terms of BOD, indicating 1,3-butadiene is not readily biodegradable with a half-life greater than 28 days (NITE, 2020). Based on EPI Suite™ modeling, 1,3-butadiene biodegradation is expected to be 2.82 days in aerobic environments (BioHCwin estimated half-life). Notably, OECD 301D Ready Biodegradability Tests are conducted in closed systems which are not representative of the natural environment with continuous chemical movement. Details on the experimental conditions of the OECD 301D equivalent test were not recorded, making the interpretation of the results difficult. Anaerobic biodegradation in water was estimated to have a half-life of 4 – 16 weeks (NCBI, 2020; Howard et al., 1991). 1,3-Butadiene is thought to degrade to form carbon dioxide and acetate (Watkinson and Somerville, 1976). It has also been shown to be oxidized to form 1,2-epoxybutene by methane-utilizing bacteria (Hou et al., 1979).

3.4.2 Photodegradation

Direct photolysis of 1,3-butadiene in air is assumed to be an insignificant process relative to photooxidation reactions (NCBI, 2020; ATSDR, 2012; ECB, 2002) because 1,3-butadiene does not contain chromophores that absorb light at wavelengths exceeding 290 nm. Indirect photolysis of 1,3-butadiene in surface waters is also expected to be an insignificant pathway though it has been estimated to range from 50 to 2,000 days (Howard et al., 1991).

Indirect photodegradation of 1,3-butadiene in air is a significant pathway. 1,3-Butadiene will degrade in air rapidly during the day (half-life = 1.6–2.6 hours) by reacting with photochemically-produced hydroxyl radicals in the atmosphere (Khaled et al., 2019; Vimal, 2008; Klamt, 1993). Measured and estimated average atmospheric half-lives for photodegradation of 1,3-butadiene range from 0.76 to 9 hours and is dependent on daylight (ECB, 2002; Howard et al., 1991; Andersson and Ljungström, 1989). Specifically, assuming 12 hours of daylight and hydroxyl radical concentration of 1.5×10^6 OH molecules/cm^3, 1,3-butadiene half-life is 1.6 to 2.6 hours (Khaled et al., 2019; Vimal, 2008; Klamt, 1993). Nitrate radicals destroy 1,3-butadiene in the absence of light (night) (Andersson and Ljungström, 1989). 1,3-Butadiene will react with nitrate radicals with a half-life ranging from 5 to 9 hours (Zhao et al., 2011; Andersson and Ljungström, 1989) and ozone with a half-life of 34 hours (U.S. EPA, 2012a). Reaction with ozone is not expected to expedite indirect photodegradation of 1,3-butadiene in the atmosphere.

Many transformation products are formed from the indirect photodegradation of 1,3-butadiene by reaction with hydroxyl radicals, ozone, and nitrate radicals. The main transformation products are formaldehyde and acrolein. Additional transformation products formed in the atmosphere in lesser amounts include furan, 1,3-butadiene monoxide, 1,3-butadiene diepoxide, organic nitrates, glycolaldehyde, glycidaldehyde, 3-hydroxy-propanaldehyde, hydroxy acetone, and malonaldehyde (Ghosh et al., 2010; Sexton et al., 2007; Liu et al., 1999; Tuazon et al., 1999). Tuazon et al., (1999) found that molar yields of 58 and 62 percent for acrolein and formaldehyde, respectively, were formed from the reaction of 1,3-butadiene with hydroxyl radicals in the atmosphere. Two outdoor smog chamber experiments found that during atmospheric photodegradation—about 25 percent of 1,3-butadiene formed acrolein (Sexton et al., 2007; Liu et al., 1999) while 7 to 8 percent formed formaldehyde (Sexton et al., 2007). Sexton et al., (2007) attributed the low transformation percentages to the fact that both formaldehyde and acrolein are highly reactive themselves and are eventually consumed in the smog chamber experiment when 1,3-butadiene ceases to be replenished. The SAPRC-99 chemical mechanism, which is a detailed mechanism for the gas-phase atmospheric reactions of volatile organic compounds and oxides of nitrogen in in urban and regional atmospheres (Carter, 2000), estimates approximately 50 percent formation of formaldehyde when 1,3-butadiene reacts with hydroxyl radical (·OH) in the atmosphere. Ghosh et al., (2010) estimated a yield of 63 percent for both formaldehyde and acrolein when 1,3-butadiene reacts with hydroxyl radicals.

3.5 Media Assessments

3.5.1 Air and Atmosphere

1,3-Butadiene is reactive in air with an estimated half-life of 0.76 to 9 hours (Table 3-1). In daylight, reaction with hydroxyl radicals is rapid. At night, reaction with nitrate radicals become more important than reaction with hydroxyl radicals. Ozone reaction (half-life of 34 hours) is less important than reaction with hydroxyl radicals (ECB, 2002). 1,3-Butadiene is not expected to undergo air deposition nor long-range transport based on a low log K_{OA} of 1.5 and a short half-life in the atmosphere. The OECD Overall Environmental Persistence (POV) and long-range transport potential (LRTP) Screening Tool, Version 2.2 (Wegmann et al., 2009) was used to estimate potential for long range transport. It estimates a Characteristic Travel Distance (CTD) of 187 km, and Transfer Efficiency (TE) of 3.23×10^{-6} percent when reported releases are made solely to air. A molecular mass of 54.09 g/mol, log K_{AW} of 0.492, and log K_{OW} of 1.99 along with atmospheric half-life of 9 hours, water half-life of 28 days, and soil half-life of 28 days were used in the analysis. The CTD is the distance from the point of release of the chemical to the point at which the concentration of the chemical has dropped to about 37 percent of its initial value, while the TE estimates the percentage of emitted chemical that is deposited to surface media after transport away from the region of release. A CTD of 187 km suggests that 1,3-butadiene is

not likely to undergo long-range transport in the air and a TE of 3.23×10^{-6} percent suggests that a negligible amount of 1,3-butadiene emitted to air will be deposited to surface media after transport away from the region of release. Results showed that neither long range transport nor air deposition is a concern for 1,3-butadiene. Monitoring concentrations of 1,3-butadiene in air across the United States documented in the AMTIC archive (U.S. EPA, 2019a) range from non-detect to 267.3 µg/m^3. More details of monitoring data can be found in the *Draft Environmental Media Concentrations for 1,3-Butadiene* (U.S. EPA, 2024c).

3.5.2 Aquatic Environments

1,3-Butadiene in surface water is expected to volatilize rapidly given its physical and chemical properties (Table 2-1). EPI Suite™ estimated volatilization half-life from water ranged from 0.76 hours in a model river to 2.9 days in a model lake. These volatilization half-lives are based on a depth of 1 m, wind velocity of 5 m/s and current velocity of 1 m/s for the model river and a depth of 1 m, wind velocity of 0.5 m/s and current velocity of 0.05 m/s for the model lake. Other inputs to EPI Suite™ are listed in (Table 2-1).

According to estimated half-lives, biodegradation is expected to be fast in aerobic sediments and slower under anaerobic conditions; however, volatilization. is expected to be the most important removal process for 1,3-butadiene in aquatic environments. Further, due to high volatility and low sorption potential to organic matter (Table 2-1), 1,3-butadiene is not expected to significantly partition into sediments in water. 1,3-Butadiene does not undergo hydrolysis and indirect photolysis is expected to be an insignificant process of removal from surface waters (NCBI, 2020; Howard et al., 1991). 1,3-Butadiene was not detected in surface water across the United States based on available monitoring data documented in the Water Quality Portal (WQP) (U.S. EPA, 2022). More details on monitoring data can be found in the *Draft Environmental Media Concentrations for 1,3-Butadiene* (U.S. EPA, 2024c).

3.5.3 Terrestrial Environments

According to the TSCA conditions of use for 1,3-butadiene, it is not expected to be released to soil. Although air deposition to soil may occur, it is not expected to be significant (see Section 3.3.1) and due to the physical and chemical properties of 1,3-butadiene (Table 2-1), it is expected to volatilize rapidly from soil and other surfaces. Further, there is low potential for sorption to organic matter in soil (K_{OC} = 53.7). The estimated half-life of 1,3-butadiene in soil ranges from 7 to 28 days.

TRI (U.S. EPA, 2019c) reported relatively low releases of 1,3-butadiene to wastewater treatment systems (U.S. EPA, 2024d) and the Clean Water Act Discharge Monitoring Reports (DMR) (U.S. EPA, 2019b) recorded no releases of 1,3-butadiene from wastewater treatment plants to surface water bodies for the period between 2016 and 2021. As a result, the EPA does not anticipate 1,3-butadiene to be present in biosolids because of low releases of 1,3-butadiene to wastewater treatment systems, low potential for sorption to organic matter, and high volatility.

Because releases to landfills are expected to be mostly in polymer form from which depolymerization and subsequent exposure to 1,3-butadiene monomer is not expected, 1,3-butadiene in landfills is not expected to be a source of soil or groundwater contamination. Although the K_{OC} (53.7) and K_{OW} (97.7) values for 1,3-butadiene suggest it will be relatively mobile in groundwater, current release patterns (low releases to land and water) and the volatility of 1,3-butadiene make it unlikely for 1,3-butadiene to be present in groundwater. Available monitoring data documented in the WQP (U.S. EPA, 2022) for groundwater across the United States reveals 99 percent non-detects of 9,378 samples collected between 2011 and 2023. Concentrations of 1,3-butadiene in groundwater range from non-detect to 40 µg/l. More details of monitoring data can be found in the *Draft Environmental Media Concentrations for 1,3-*

Butadiene (U.S. EPA, 2024c).

3.6 Persistence Potential of 1,3-Butadiene

1,3-Butadiene is not likely to persist in the environment due to the rapid volatilization from water and surfaces and the reactivity in the atmosphere. Based on results from BIOWIN™, which is an EPI Suite™ model that estimates the probability of rapid aerobic and anaerobic biodegradation of an organic compound in the presence of mixed populations of environmental microorganisms, biodegradation is expected to be fast in aerobic aquatic environments and slow in anaerobic aquatic environments. BioHCwin™, which is an EPI Suite™ model specifically developed for the biodegradation half-life prediction of petroleum hydrocarbons, estimated a half-life of 2.82 days for 1,3-butadiene in an aerobic aquatic environment. This short half-life agrees with the BIOWIN™ results that aerobic biodegradation is expected to be rapid in aquatic environments. Volatilization half-life from water is estimated to range from 0.76 hours in rivers to 2.9 days in lakes. Further, there is fast reaction with hydroxyl radicals ($t_{1/2}$ = 0.161 days, AOPWIN) and ozone ($t_{1/2}$ = 1.415 days, AOPWIN) in air. These metrics suggest 1,3-butadiene is not likely to be persistent in the environment.

3.6.1 Destruction and Removal Efficiency

Incineration of waste 1,3-butadiene from industrial activities is expected to occur at hazardous waste incinerators at a Destruction and Removal Efficiency (DRE) of greater or equal to 99.99 percent (ECB, 2002).

The Clean Air Act 40CFR Part 63, Subpart EEE—National Emission Standards for Hazardous Air Pollutants from Hazardous Waste Combustors—requires all hazardous waste combustors, hazardous waste incinerators, hazardous waste cement kilns, hazardous waste lightweight aggregate kilns, hazardous waste solid fuel boilers, hazardous waste liquid fuel boilers, and hazardous waste hydrochloric acid production furnaces to achieve a destruction and removal efficiency (DRE) of 99.99 percent for each principle organic hazardous constituent (POHC)—including 1,3-butadiene.

3.6.2 Removal in Wastewater Treatment

Due to the volatility of 1,3-butadiene, only small amounts are expected to enter wastewater treatment plants (WWTPs). The small amounts that enter a WWTP are expected to be removed primarily by volatilization and possibly some biodegradation. Based on its low potential for sorption to organic matter, sorption to sludge is not expected to be a significant removal route for 1,3-butadiene in WWTPs.

The EPI Suite™ (U.S. EPA, 2012a) STPWIN model was run using default settings (biodegradation half-life was set to 10,000 hours to evaluate degradation based on abiotic processes alone) and 1,3-butadiene physical and chemical properties outlined in Table 2-1 to evaluate its potential to volatilize to air or adsorb to sludge during wastewater treatment. EPI Suite™ STPWIN modeling estimated 96.25 percent removal via volatilization, 0.53 percent removal via sludge adsorption, and 3.2 percent loss to effluent—further highlighting that volatilization is the primary pathway for environmental fate of 1,3-butadiene.

3.6.3 Bioaccumulation Potential of 1,3-Butadiene

Based on its reactivity, 1,3-butadiene is not expected to bioaccumulate or bioconcentrate. There were no available data identified in systematic review evaluating bioaccumulation of 1,3-butadiene in aquatic or terrestrial environments. The EPI Suite™ (U.S. EPA, 2012a) BCFBAF model indicated low potential for 1,3-butadiene bioaccumulation in the environment with an estimated log BCF of 0.98. The bioconcentration factor regression-based estimate was 9.55 L/kg wet-weight and the biotransformation half-life normalized to 10 g fish was 0.34 days.

4 OVERALL FATE AND TRANSPORT OF 1,3-BUTADIENE

With approximately 98 percent of 1,3-butadiene released to air as reported by TRI (*Draft Environmental Release for 1,3-Butadiene* (U.S. EPA, 2024d)), air is expected to be the primary major environmental compartment for 1,3-butadiene. It will degrade in daylight rapidly (half-life of 1.6–2.6 hours) by reaction with photochemically-produced hydroxyl radicals in the atmosphere. It will also react at a much slower rate with nitrate radicals and ozone in the atmosphere (half-lives of 3–9 and 34 hours, respectively). Based on an estimated octanol-air partition coefficient (K_{OA}) of 31.5 to 33.7, 1,3-butadiene is not expected to associate strongly with airborne particulates; hence, it is not expected to undergo dry deposition or long-range transport in air. It is expected to remain largely in the vapor phase where it will undergo photodegradation. 1,3-Butadiene is not expected to persist in air due to its reactivity and multiple degradation pathways.

DMRs recorded no releases of 1,3-butadiene from WWTPs to surface water bodies for the time between 2016 and 2021, though TRI reported small releases to water (U.S. EPA, 2024d). Hydrolysis in environmental waters is not expected to be a significant process for 1,3-butadiene based on its lack of hydrolyzable functional groups. The aerobic biodegradation half-life of 1,3-butadiene in water is expected to fall in the range of 7 to 28 days while anaerobic biodegradation in water was estimated to have a half-life of 4 to 16 weeks. Based on the reported rates, biodegradation of 1,3-butadiene in environmental water is likely less important than volatilization. Volatilization from water is expected to be a significant process for 1,3-butadiene based on a high Henry's Law constant (0.076 atm·m^3/mol at 25 °C) and a high vapor pressure (1,900 mm Hg at 20 °C); thus, mitigating its presence or persistence in aquatic environments. 1,3-Butadiene is not expected to bioaccumulate in aquatic organisms given its estimated BCF of 9.55 L/kg.

Overall, 1,3-butadiene is primarily released to, and will generally partition to, air where it has low persistence potential. Figure 4-1 below is a pictorial description of the fate and transport of 1,3-butadiene in the environment.

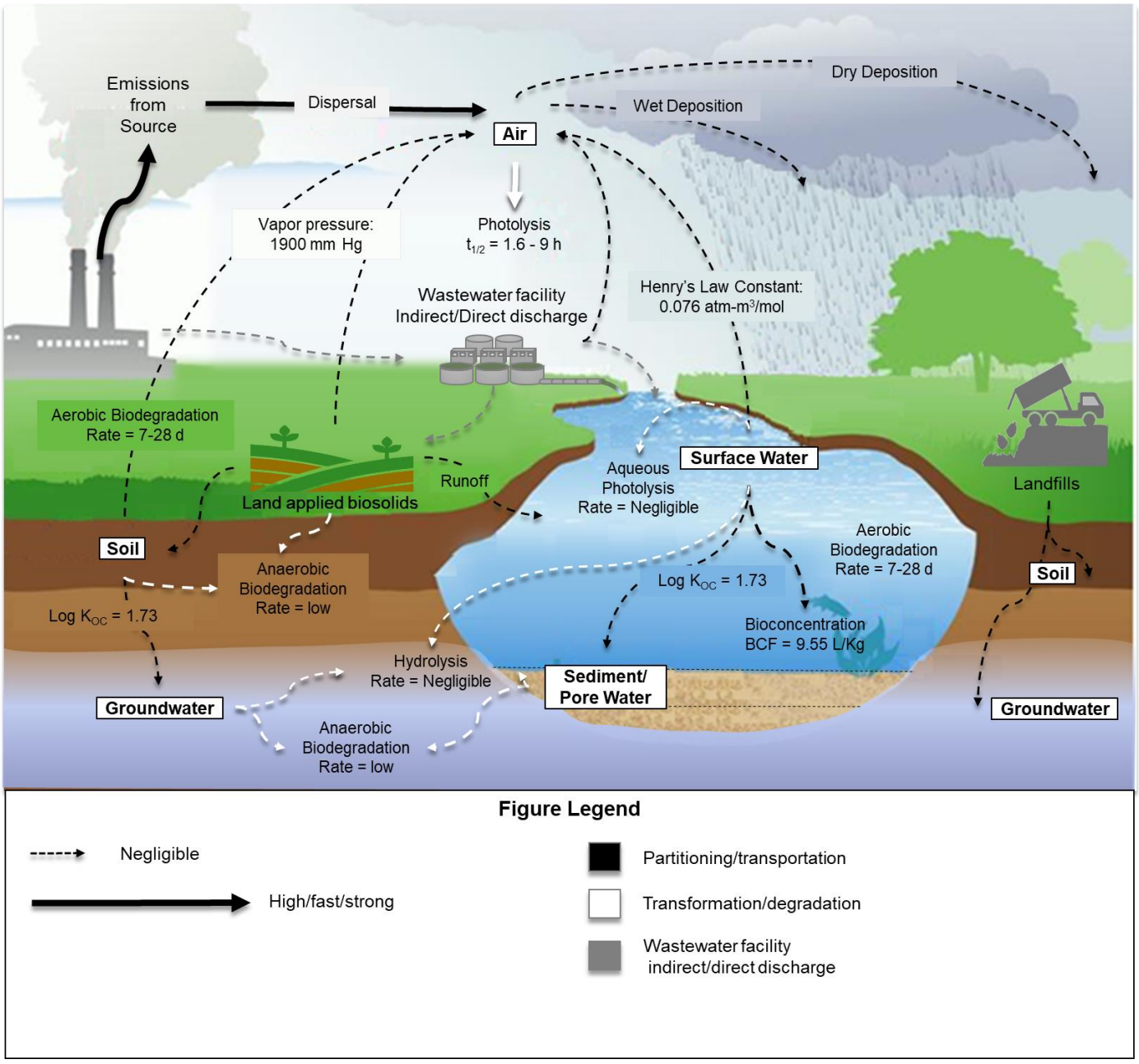


Figure 4-1. Transport, Partitioning and Degradation of 1,3-Butadiene in the Environment
The diagram depicts the distribution (grey arrows), transport and partitioning (black arrows) as well as the transformation and degradation (white arrows) of 1,3-butadiene in the environment. The width of the arrow is a qualitative indication of the likelihood that the indicated partitioning will occur or the rate at which the indicated degradation will occur (*i.e.*, wider arrows indicate more likely partitioning or more rapid degradation).

5 WEIGHT OF SCIENTIFIC EVIDENCE CONCLUSIONS FOR 1,3-BUTADIENE

5.1 Weight of Scientific Evidence Conclusions for Physical and Chemical Properties

The general confidence in the physical and chemical properties for 1,3-butadiene is high. Measured data were identified from high-quality studies for all physical and chemical properties. A detailed discussion of strengths, limitations, assumptions, and key sources of uncertainty for the fate and transport assessment is provided below.

5.1.1 Strengths, Limitations, Assumptions, and Key Sources of Uncertainty for the Physical and Chemical Property Assessment

The physical and chemical property data discussed in this document were the product of a systematic review of reasonably available information (U.S. EPA, 2024h). Overall, there is little uncertainty in the physical and chemical data and analyses presented and there is high confidence in the data. The analyses present the average and standard deviation of all data collected through the systematic review process for each parameter. The standard deviation is reported as uncertainty in the form of tolerance limits (± range) on the average value. Data extracted as a range of values were excluded from the calculations unless expert judgment could identify precise data points within the range. These statistical analyses may be indicative of the amount of uncertainty related to different instrumental techniques or other experimental differences between the studies used to generate the data. Additional sources of uncertainty in these reported values may be inherent to the measurement of the data point itself (*e.g.*, sources of uncertainty or measurement error related to the instrumental method, precision with which a data point is measured and reported in the data source). Finally, all data was assumed to be collected under standard environmental conditions (*i.e.*, 20–25 °C and 760 mmHg) unless otherwise specified.

Due to cross-referencing between many of the databases identified and assessed through the systematic review process, there is potential for data from one primary source to be collected multiple times, resulting in duplication within the dataset. This duplication should be considered a potential source of uncertainty in the data analyses; however, data-curation procedures and expert judgement were used to minimize this possibility whenever possible.

5.2 Weight of Scientific Evidence Conclusions for Fate and Transport

Evaluation of the Weight of the Scientific Evidence for the fate and transport of 1,3-butadiene is shown below and is based on categorization described in the 2021 Draft Systematic Review Protocol Supporting TSCA Risk Evaluations (U.S. EPA, 2021).

There is robust evidence showing that 1,3-butadiene will

- photodegrade rapidly in air to yield formaldehyde and acrolein (Section 3.4.2);
- not partition to organic matter in water (Section 3.5.2); and
- not hydrolyze significantly in water (Section 3.5.2).

There is moderate evidence showing that 1,3-butadiene will

- biodegrade rapidly in aerobic river water or wetland sediment (Section 3.4.1);
- biodegrade rapidly in aerobic soil (Section 3.4.1);
- not sorb to soil/sediment particles (Section 3.5.3);
- not biodegrade rapidly in anaerobic sediment (Section 3.4.1);

- biodegrade in soil or water to give carbondioxide and acetate (Section 3.4.1);
- be degraded by methane-utilizing bacteria to form 1,2-epoxybutene (Section 3.4.1); and
- not bioaccumulate in fish (Section 3.6.3).

5.2.1 Strengths, Limitations, Assumptions, and Key Sources of Uncertainty for the Fate and Transport Assessment

Due to the high reactivity and volatilization of 1,3-butadiene, there are few high-quality studies evaluating environmental fate. Measured data were identified from high-quality studies for indirect photodegradation of 1,3-butadiene in the atmosphere; however, there is generally limited evidence on the fate of 1,3-butadiene in the environment. This lack of data creates some uncertainty. Nevertheless, EPA has high confidence in our assumptions about the fate of 1,3-butadiene in the environment based on its physical and chemical properties, environmental release data and monitoring data.

Half-lives of 1,3-butadiene in air can vary significantly under different environmental conditions, which result in spatio-temporal variation in degradation rates that contribute to uncertainty. For instance, greater residence times of 1,3-butadiene are expected in colder, cloudy conditions.

The fate assessment of 1,3-butadiene in aquatic environments was based mainly on physical and chemical data and estimated properties and release data. Volatilization and biodegradation are key processes in the fate of 1,3-butadiene in water; however, no available data was found measuring the volatilization of 1,3-butadiene from water and sediments. There was only one reference with measured data for biodegradation of 1,3-butadiene in water and no data were identified for biodegradation in sediments which is a source of uncertainty. Estimations of volatilization using EPI Suite™ are based on a shallow model river and lake and may be much lower for deeper water bodies.

Like aquatic environments, experimental data for the fate of 1,3-butadiene in terrestrial environments were not identified through systematic review. This is a source of uncertainty. However, EPA relied on release data, monitoring data and the physical and chemical properties to conduct the fate assessment for 1,3-butadiene and are confident that exposures are not being underestimated.

Although there are no measured data of potential bioaccumulation of 1,3-butadiene, there is high confidence in the assumption that bioaccumulation potential is minimal. Given the high reactivity of 1,3-butadiene and the log K_{ow} of 1.99, it is not expected to persist in the environment long enough to support potential bioaccumulation. Thus, the uncertainty is minimal and there is high confidence that 1,3-butadiene will not bioaccumulate in aquatic or terrestrial species.

6 CONCLUSIONS

Based on the high release amounts of 1,3-butadiene to the atmosphere, air is expected to be a major pathway of exposure. Low release amounts to water as well as high volatility means the water pathway is not expected to be a significant pathway of exposure. Sediments and soil are also not expected to be major pathways for 1,3-butadiene based on low partition coefficients to organic matter (K_{OW}, K_{OC}, and K_{OA}) and a significant water solubility. Bioaccumulation in biota is low so trophic transfer is not expected to be a concern. These conclusions are supported by available monitoring data.

Based on the forgoing conclusions, the human health assessment will focus primarily on inhalation risk to the general population and workers from exposure to 1,3-butadiene in air (U.S. EPA, 2024e). The assessment of risk to terrestrial and aquatic organisms due to 1,3-butadiene exposure will be handled qualitatively because exposure is not expected from the soil and water pathways (U.S. EPA, 2024g).

7 REFERENCES

Andersson, Y; Ljungström, E. (1989). Gas phase reaction of the NO3 radical with organic compounds in the dark. Atmos Environ (1967) 23: 1153-1155. http://dx.doi.org/10.1016/0004-6981(89)90316-8

ATSDR (Agency for Toxic Substances and Disease Registry). (2012). Toxicological profile for 1,3-butadiene [ATSDR Tox Profile]. Atlanta, GA: U.S. Department of Health and Human Services, Public Health Service. http://www.atsdr.cdc.gov/toxprofiles/tp.asp?id=459&tid=81

Carter, WPL. (2000). Implementation of the SAPRC-99 chemical mechanism into the Models-3 framework. Sacramento, CA: California Air Resources Board (CARB).

ECB (European Chemicals Bureau). (2002). European Union risk assessment report: 1,3-butadiene. Luxembourg: European Union, European Chemicals Bureau, Institute for Health and Consumer Protection. https://echa.europa.eu/documents/10162/1f512549-5bf8-49a8-ba51-1cf67dc07b72

Ghosh, B; Bugarin, A; Connell, BT; North, SW. (2010). OH radical initiated oxidation of 1,3-butadiene: isomeric selective study of the dominant addition channel. J Phys Chem A 114: 5299-5305. http://dx.doi.org/10.1021/jp1006878

Hou, CT; Patel, R; Laskin, AI. (1979). Microbial oxidation of gaseous hydrocarbons: Epoxidation of C2 to C4 n-alkenes by methylotrophic bacteria. Appl Environ Microbiol 38: 127-134.

Howard, PH; Boethling, RS; Jarvis, WF; Meylan, WM; Michalenko, EM. (1991). Handbook of environmental degradation rates. In PH Howard (Ed.), (pp. 3). Boca Raton, FL: Lewis Publishers/CRC Press. http://www.crcpress.com/product/isbn/9780873713580

Kerns, M; Henning, S; Rachita, M. (2002). Butadiene polymers. In HF Mark (Ed.), Encyclopedia of polymer science and technology, vol 5 (pp. 317-356). New York, NY: Wiley. http://dx.doi.org/10.1002/0471440264.pst034

Khaled, F; Giri, BR; Liu, D; Assaf, E; Fittschen, C; Farooq, A. (2019). Insights into the Reactions of Hydroxyl Radical with Diolefins from Atmospheric to Combustion Environments. J Phys Chem A 123: 2261-2271. http://dx.doi.org/10.1021/acs.jpca.8b10997

Klamt, A. (1993). Estimation of gas-phase hydroxyl radical rate constants of organic compounds from molecular orbital calculations. Chemosphere 26: 1273-1289. http://dx.doi.org/10.1016/0045-6535(93)90181-4

Liu, X; Jeffries, HE; Sexton, KG. (1999). Hydroxyl radical and ozone initiated photochemical reactions of 1,3-butadiene. Atmos Environ 33: 3005-3022. http://dx.doi.org/10.1016/S1352-2310(99)00078-3

National Toxicology Program (NTP). (1993). NTP technical report on the toxicology and carcinogenesis studies of 1,3-butadiene (CAS no. 106-99-0) in B6C3F1 mice (inhalation studies). (blication No 93-3165). Research Triangle Park, NC: U.S. Department of Health and Human Services, National Institutes of Health, National Toxicology Program. https://ntp.niehs.nih.gov/ntp/htdocs/lt_rpts/tr434.pdf

NCBI (National Center for Biotechnology Information). (2020). PubChem database: compound summary: 1,3-butadiene. Available online at https://pubchem.ncbi.nlm.nih.gov/compound/1_3-Butadiene

NIST (National Institute of Standards and Technology). (2022). NIST Chemistry WebBook. 1,3-Butadiene (106-99-0). Standard Reference Database No. 69. Washington, DC: US Sec Commerce. https://webbook.nist.gov/cgi/cbook.cgi?ID=106-99-0&Units=SI&cTG=on&cIR=on&cTC=on&cTZ=on&cTP=on&cMS=on&cTR=on&cUV=on&cIE=on&cGC=on&cIC=on&cES=on&cDI=on&cSO=on

NITE (National Institute of Technology and Evaluation). (2020). Biodegradation of 1,3-butadiene in water: Screening tests. Tokyo, Japan: Japanese Ministry of the Environment. https://www.nite.go.jp/chem/jcheck/template.action?ano=2866&mno=2-0017&cno=106-99-0&request_locale=en

NLM (National Library of Medicine). (2003). PubChem: Hazardous Substance Data Bank: 1,3-Butadiene, 106-99-0. Available online at

O'Neil, MJ. (2013). 1,3-Butadiene. 106-99-0. In MJ O'Neill; PE Heckelman; PH Dobbelaar; KJ Roman; CM Kenney; LS Karaffa (Eds.), The Merck index (15th ed., pp. 267). Cambridge, UK: The Royal Society of Chemistry.

OEHHA, COoEHHA. (2014). Appendix D: Individual acute, 8-hour, and chronic reference exposure level summaries. Sacramento, CA: Office of Environmental Health Hazard Assessment, California EPA. https://oehha.ca.gov/media/downloads/crnr/appendixd1final.pdf

Rumble, JR. (2018a). Aqueous solubility and Henry's law constants of organic compounds. In CRC Handbook of Chemistry and Physics (99 ed.). Boca Raton, FL: CRC Press. Taylor & Francis Group. https://hbcp.chemnetbase.com/faces/documents/05_32/05_32_0001.xhtml

Rumble, JR. (2018b). 1,2-dichlorobenzene. In JR Rumble (Ed.), CRC handbook of chemistry and physics (99th ed., pp. 3-16). Boca Raton, FL: CRC Press.

Rumble, JR, (Ed.). (2018c). 1,3-Butadiene. In CRC handbook of chemistry and physics (99 ed.). Boca Raton, FL: CRC Press. Taylor & Francis Group.

Rumble, JR; Lide, DR; Bruno, TJ. (2018). Octanol-water partition coefficients. In JR Rumble; DR Lide; TJ Bruno (Eds.), CRC handbook of chemistry and physics (99th ed., pp. 5-148-145-187). Boca Raton, FL: CRC Press.

SAB (Science Advisory Board). (2007). Science Advisory Board (SAB) review of the Estimation Programs Interface Suite (EPI Suite). (EPA-SAB-07-11). Washington, DC: U.S. Environmental Protection Agency.

Sexton, KG; Doyle, ML; Jeffries, HE; Ebersviller, S. (2007). Development and testing of a chemical mechanism for atmospheric photochemical transformations of 1,3-butadiene. Chem Biol Interact 166: 156-162. http://dx.doi.org/10.1016/j.cbi.2007.01.002

Sun, HN; Wristers, JP. (2002). Butadiene. In Kirk-othmer encyclopedia of chemical technology (1999-2013). New York, NY: John Wiley & Sons. http://dx.doi.org/10.1002/0471238961.02212001192114.a01.pub2

Tuazon, EC; Alvarado, A; Aschmann, SM; Atkinson, R; Arey, J. (1999). Products of the gas-phase reactions of 1,3-butadiene with OH and NO3 radicals. Environ Sci Technol 33: 3586-3595. http://dx.doi.org/10.1021/es990193u

U.S. EPA (U.S. Environmental Protection Agency). (2012a). Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11 [Computer Program]. Washington, DC. Retrieved from https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface

U.S. EPA (U.S. Environmental Protection Agency). (2012b). PhysProp database. Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11: Formaldehyde (CASRN: 50-00-0) [Fact Sheet]. Washington, DC. https://www.epa.gov/tsca-screening-tools/epi-suitetm-estimation-program-interface

U.S. EPA (U.S. Environmental Protection Agency). (2019a). AMTIC Ambient Monitoring HAPs Data by Year: 1,3-Butadiene (2015-2019). Washington, DC. Retrieved from https://www.epa.gov/amtic/amtic-ambient-monitoring-archive-haps

U.S. EPA (U.S. Environmental Protection Agency). (2019b). Discharge Monitoring Report (DMR) data, Reporting year 2019: 1,3-Butadiene (CAS RN 106-99-0). Washington, DC. Retrieved from https://echo.epa.gov/trends/loading-tool/water-pollution-search

U.S. EPA (U.S. Environmental Protection Agency). (2019c). TRI Explorer, Reporting year 2019: 1,3-Butadiene (CAS RN 106-99-0). Washington, DC. Retrieved from https://echo.epa.gov/trends/loading-tool/water-pollution-search

U.S. EPA (U.S. Environmental Protection Agency). (2020). Final scope of the risk evaluation for 1,3-butadiene; CASRN 106-99-0. (EPA 740-R-20-011). Washington, DC: Office of Chemical Safety and Pollution Prevention. https://www.epa.gov/sites/default/files/2020-09/documents/casrn_106-

99-0_13-butadiene_finalscope.pdf
U.S. EPA (U.S. Environmental Protection Agency). (2021). Draft systematic review protocol supporting TSCA risk evaluations for chemical substances, Version 1.0: A generic TSCA systematic review protocol with chemical-specific methodologies. (EPA Document #EPA-D-20-031). Washington, DC: Office of Chemical Safety and Pollution Prevention. https://www.regulations.gov/document/EPA-HQ-OPPT-2021-0414-0005
U.S. EPA (U.S. Environmental Protection Agency). (2024a). Draft Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.
U.S. EPA (U.S. Environmental Protection Agency). (2024b). Draft Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.
U.S. EPA (U.S. Environmental Protection Agency). (2024c). Draft Environmental Media Concentrations for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.
U.S. EPA (U.S. Environmental Protection Agency). (2024d). Draft Environmental Release for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.
U.S. EPA (U.S. Environmental Protection Agency). (2024e). Draft Human Health Hazard Assessment for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.
U.S. EPA (U.S. Environmental Protection Agency). (2024f). Draft Occupational Exposure Assessment for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.
U.S. EPA (U.S. Environmental Protection Agency). (2024g). Draft Risk Evaluation for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.
U.S. EPA (U.S. Environmental Protection Agency). (2024h). Draft Systematic Review Protocol for 1,3-Butadiene. Washington, DC: Office of Pollution Prevention and Toxics.
U.S. EPA, USGS, National Water Quality Monitoring Council. (2022). 1,3-Butadiene (BTD) (CAS RN: 106-99-0): WQP Output (NWIS, STEWARDS & STORET), Site data & sample results (physical/chemical metadata) [Database]: National Water Quality Monitoring Council. Retrieved from https://acwi.gov/monitoring/waterqualitydata.html
Vimal, D. (2008) Laboratory investigations of the hydroxyl radical-initiated oxidation of atmospheric volatile organic compounds. (Doctoral Dissertation). Indiana University, Bloomington, IN.
Watkinson, RJ; Somerville, HJ. (1976). The microbial utilization of butadiene. In Proceedings of the Third International Biodegradation Symposium London. London: Applied Science Publishers.
Wegmann, F; Cavin, L; Macleod, M; Scheringer, M; Hungerbuhler, K. (2009). The OECD software tool for screening chemicals for persistence and long-range transport potential. Environ Modell Softw 24: 228-237. http://dx.doi.org/10.1016/j.envsoft.2008.06.014
Zhao, Z; Husainy, S; Smith, GD. (2011). Kinetics studies of the gas-phase reactions of NO3 radicals with series of 1-alkenes, dienes, cycloalkenes, alkenols, and alkenals. J Phys Chem A 115: 12161-12172. http://dx.doi.org/10.1021/jp206899w