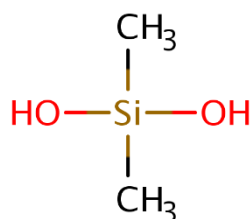


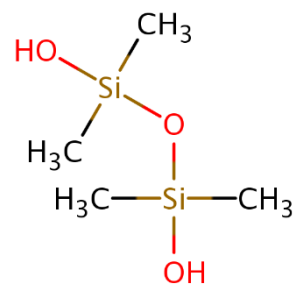


## Final Scope of Risk Evaluation for Octamethylcyclotetra- siloxane (D4)

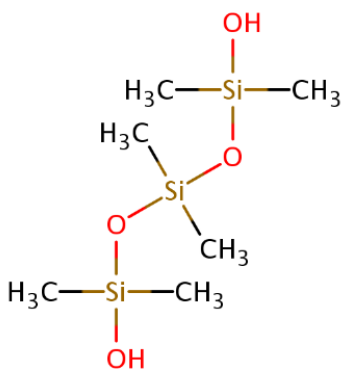
### Supplemental File: Data Extraction and Data Evaluation Tables for Physical and Chemical Property Studies for D4 Degradants



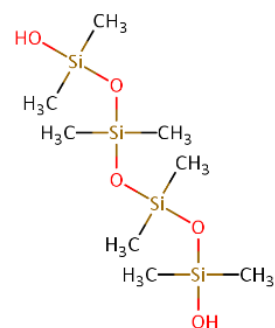
(CASRN 1066-42-8)



(CASRN 1118-15-6)



(CASRN 3663-50-1)



(CASRN 3081-07-0)

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## Dimethylsilanediol (CASRN 1066-42-8) Data Extraction Tables

Table 1. Physical State Study Summary

Study Type	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	2 values reported in Reaxys; crystal phase – interplanar spacing and leafs		( <a href="#">Elsevier, 2021c</a> )	High

Table 2. Physical Properties Study Summary

No Physical Properties data were identified for this chemical.

Table 3. Melting Point Study Summary

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	94.5–101 °C	10 values reported in Reaxys; the test substance was dissolved in a solvent for 6 values. Decomposition was reported at 99–100 °C.	( <a href="#">Elsevier, 2021c</a> )	High

Table 4. Boiling Point Study Summary

No Boiling Point data were identified for this chemical.

Table 5. Density Study Summary

Study Type	Study Details	Reference Substance	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental				1.095–1.099 g/cm <sup>3</sup>	1 value reported in Reaxys	( <a href="#">Elsevier, 2021c</a> )	High
Experimental				0.97 g/mL	NR	( <a href="#">RSC, 2021</a> )	Medium

Table 6. Vapor Pressure Study Summary

No Vapor Pressure data were identified for this chemical.

Table 7. Vapor Density Study Summary

No Vapor Density data were identified for this chemical.

Table 8. Water Solubility Study Summary

Study Type	Substance Purity	Temperature	pH	Analytical Method	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	25 °C	NR		2450 g/L	2 values reported in Reaxys; temperature reported for one value only	( <a href="#">Elsevier, 2021c</a> )	High
Experimental	NR	NR	NR		11.0 M	Equivalent to 1,010,000 mg/L based on MW 92.17 g/mol	( <a href="#">U.S. EPA, 2021b</a> )	High
Experimental	NR	NR	NR		10.8 M	Equivalent to 995,000 mg/L based on MW 92.17 g/mol	( <a href="#">U.S. EPA, 2021b</a> )	High
Experimental	NR	NR	NR		10.85 M	Equivalent to 117.7 mg/L based on MW 92.17 g/mol	( <a href="#">NLM, 2021b</a> )	High

Table 9. Octanol Water Coefficient (logKow) Study Summary

Study Type	Substance Purity	Temperature	pH	Other Study Details (Amounts of Substance Liquid Phases)	Result	Comments	Affiliated References	Data Quality Evaluation Results
Experimental	NR	20.1	NR	NR	-0.41±0.10	1 value reported in Reaxys	( <a href="#">Elsevier, 2021c</a> ) and ( <a href="#">Xu and Kropscott, 2012</a> )	High

Table 10. Henry's Law Constant Study Summary

Study Type	Substance Purity	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	98.1% radiochemical purity	20.1 °C	-6.84	$\log K_{aw} = -6.84 \pm 0.34$ ; Air = $1 \times 10^{-5}$ mg/L; Water = 70.0 mg/L	( <a href="#">Xu and Kropscott, 2012</a> )	High

Table 11. Flash Point Study Summary

No Flash Point data were identified for this chemical.

Table 12. Auto Flammability Study Summary

No Autoflammability data were identified for this chemical.

Table 13. Viscosity Study Summary

No Viscosity data were identified for this chemical.

Table 14. Refractive Index Study Summary

Study Type	Apparatus	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	25 °C	1.444–1.456	2 values were reported in Reaxys; 1.444–1.448 (n2) and 1.452–1.456 (n1), 589.3 nm	( <a href="#">Elsevier, 2021c</a> )	High

Table 15. Dielectric Constant Study Summary

No Dielectric Constant data were identified for this chemical.



EPI Suite™ Model Outputs  
([U.S. EPA, 2012](#))

SMILES : [Si](O)(O)(C)C  
CHEM : DIMETHYLSILANEDIOL  
MOL FOR: C2 H8 O2 Si1  
MOL WT : 92.17

----- EPI SUMMARY (v4.11) -----

Physical Property Inputs:

Log Kow (octanol-water): -0.41  
Boiling Point (°C): -----  
Melting Point (°C): -----  
Vapor Pressure (mm Hg): -----  
Water Solubility (mg/L): 9.95E+005  
Henry LC (atm-m<sup>3</sup>/mole): -----

Log Octanol-Water Partition Coef (SRC):  
Log Kow (KOWWIN v1.68 estimate) = -0.41

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (°C): 184.32 (Adapted Stein & Brown method)  
Melting Pt (°C): -18.70 (Mean or Weighted MP)  
VP(mm Hg, 25 °C): 0.136 (Mean VP of Antoine & Grain methods)  
VP (Pa, 25 °C): 18.1 (Mean VP of Antoine & Grain methods)

Water Solubility Estimate from Log Kow (WSKOW v1.42):

Water Solubility at 25 °C (mg/L): 2.753E+005  
log Kow used: -0.41 (user entered)  
no-melting pt equation used  
Water Sol (Exper. database match) = 1E+006 mg/L (25 °C)  
Exper. Ref: BEILSTEIN

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 1E+006 mg/L

ECOSAR Class Program (ECOSAR v1.11):

Class(es) found:  
Neutral Organics

Henrys Law Constant (25 °C) [HENRYWIN v3.20]:

Bond Method : 1.16E-008 atm-m<sup>3</sup>/mole (1.17E-003 Pa-m<sup>3</sup>/mole)  
Group Method: Incomplete  
For Henry LC Comparison Purposes:  
User-Entered Henry LC: not entered  
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:  
HLC: 1.658E-008 atm-m<sup>3</sup>/mole (1.680E-003 Pa-m<sup>3</sup>/mole)  
VP: 0.136 mm Hg (source: MPBPVP)  
WS: 9.95E+005 mg/L (source: User-Entered)

Log Octanol-Air Partition Coefficient (25 °C) [KOAWIN v1.10]:

Log Kow used: -0.41 (user entered)

Log Kaw used: -6.324 (HenryWin est)

Log Koa (KOAWIN v1.10 estimate): 5.914

Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model): 0.7037

Biowin2 (Non-Linear Model): 0.8455

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.9955 (weeks)

Biowin4 (Primary Survey Model): 3.7148 (days-weeks)

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model): 0.4388

Biowin6 (MITI Non-Linear Model): 0.4759

Anaerobic Biodegradation Probability:

Biowin7 (Anaerobic Linear Model): 0.6769

Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):

Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 16 Pa (0.12 mm Hg)

Log Koa (Koawin est): 5.914

Kp (particle/gas partition coef. (m<sup>3</sup>/ug)):

Mackay model 1.88E-007

Octanol/air (Koa) model: 2.01E-007

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model: 6.77E-006

Mackay model: 1.5E-005

Octanol/air (Koa) model: 1.61E-005

Atmospheric Oxidation (25 °C) [AopWin v1.92]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 7.1992 E-12 cm<sup>3</sup>/molecule-sec

Half-Life = 1.486 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)

Half-Life = 17.829 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

1.09E-005 (Junge-Pankow, Mackay avg)

1.61E-005 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc: 43.89 L/kg (MCI method)

Log Koc: 1.642 (MCI method)

Koc: 0.4403 L/kg (Kow method)

Log Koc: -0.356 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 °C) [HYDROWIN v2.00]:  
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):

Log BCF from regression-based method = 0.500 (BCF = 3.162 L/kg wet-wt)

Log Biotransformation Half-life (HL) = -1.4092 days (HL = 0.03897 days)

Log BCF Arnot-Gobas method (upper trophic) = -0.037 (BCF = 0.9183)

Log BAF Arnot-Gobas method (upper trophic) = -0.037 (BAF = 0.9183)

log Kow used: -0.41 (user entered)

Volatilization from Water:

Henry LC: 1.16E-008 atm-m<sup>3</sup>/mole (estimated by Bond SAR Method)

Half-Life from Model River: 4.846E+004 hours (2019 days)

Half-Life from Model Lake: 5.287E+005 hours (2.203E+004 days)

Removal in Wastewater Treatment:

Total removal: 1.85 percent

Total biodegradation: 0.09 percent

Total sludge adsorption: 1.76 percent

Total to Air: 0.00 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount Half-Life Emissions

(percent)	(hr)	(kg/hr)	
Air	0.203	35.7	1000
Water	23.1	360	1000
Soil	76.6	720	1000
Sediment	0.0843	3.24E+003	0

Persistence Time: 679 hr

## Data Evaluation Tables

Study Reference:	Elsevier (2021). Reaxys: physical-chemical property data for dimethylsilanediol. CAS Registry Number: 1066-42-8; HERO ID: 7995011					
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Test Reliability	Reliability / Unbiased (Method Objectivity)	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	Reliability / Analytical Method	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			<b>Sum of scores:</b>	2	2	2
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1	<b>Overall Score (Rounded):</b>	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Physical State reported by this reference. Cited reference: Hyde; Journal of the American Chemical Society; vol. 75; (1953); p. 2166						

Study Reference:	Elsevier (2021). Reaxys: physical-chemical property data for dimethylsilanediol. CAS Registry Number: 1066-42-8; HERO ID: 7995011					
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated NR)	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	Reliability / Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			<b>Sum of scores:</b>	7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference.  
Cited references: Makarova et al. 2006; Kennan et al. 1999; Cella and Carpenter 1994; Harris 1963; Chrzczonowicz et al. 1960; Takiguchi 1959; Kantor 1953; Hyde 1953; Kantor 1953; Hyde 1953

<b>Study Reference:</b>		<b>Elsevier (2021). Reaxys: physical-chemical property data for dimethylsilanediol. CAS Registry Number: 1066-42-8; HERO ID: 7995011</b>				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated NR)</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			<b>Sum of scores:</b>	6	4	6
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.5	<b>Overall Score (Rounded):</b>	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Density reported by this reference.  
Cited reference: Hyde; Journal of the American Chemical Society; vol. 75; (1953); p. 2166

<b>Study Reference:</b> Rsc (2021). ChemSpider: Dimethylsilanediol. HERO ID: 799339						
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	Medium	Data is from a publicly available secondary source with references to non-peer reviewed original sources.	2	1	2
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	4	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.75	<b>Overall Score (Rounded):</b>	1.8
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	Medium

The reviewer agreed with the overall rating for the Density reported by this reference.  
Cited reference: Alfa Aesar

Study Reference: Elsevier (2021). Reaxys: physical-chemical property data for dimethylsilanediol. CAS Registry Number: 1066-42-8. HERO ID: 7995011						
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	Reliability / Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Water Solubility reported by this reference.  
Cited reference: Hyde; Journal of the American Chemical Society; vol. 75; (1953); p. 2166



Study Reference:	U.S.EPA (2021). Chemistry dashboard information for Dimethylsilanediol. CAS registry number: 1066-42-8. HERO ID: 7996867					
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	Reliability / Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Water Solubility reported by this reference. Cited reference: Kovdienko et. al. Molecular informatics 29.5 (2010): 394-406.						

Study Reference:	U.S. EPA. (2021). Chemistry dashboard information for Dimethylsilanediol. CAS registry number: 1066-42-8; HERO ID: 7996867					
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	Reliability / Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Water Solubility reported by this reference. Cited reference: Physprop						

<b>Study Reference:</b>		<b>U.S. EPA (2021). Pubchem: Dimethylsilanediol. CAS registry number: 1066-42-8. HERO ID: 7998093</b>				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	Medium	Data is from a publicly available secondary source with references to non-peer reviewed original sources.	2	1	2
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				8	5	8
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.6	<b>Overall Score (Rounded):</b>	1.6
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Water Solubility reported by this reference. Cited reference: EPA DSSTox						

<b>Study Reference:</b> Elsevier (2021). Reaxys: physical-chemical property data for dimethylsilanediol. CAS Registry Number: 1066-42-8. HERO ID: 7995011						
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Octanol Water Coefficient (logKow) reported by this reference. Cited references: Xu, Shihe; Kropscott, Bruce; Analytical Chemistry; vol. 84; nb. 4; (2012); p. 1948–1955						

Study Reference:	Xu, S. and B. Kropscott (2012). Method for simultaneous determination of partition coefficients for cyclic volatile methylsiloxanes and dimethylsilanediol. Analytical Chemistry 84(4): 1948–1955. HERO ID: 2188633					
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.	1	1	1
	Reliability / Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or another developed standard.	1	1	1
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				4	4	4
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1	<b>Overall Score (Rounded):</b>	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Octanol Water Coefficient (logKow) reported by this reference.						

<b>Study Reference:</b>		<b>Elsevier (2021). Reaxys: physical-chemical property data for dimethylsilanediol. CAS Registry Number: 1066-42-8. HERO ID: 7995011</b>				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				6	4	6
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.5	<b>Overall Score (Rounded):</b>	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Refractive Index reported by this reference. Cited reference: Hyde; Journal of the American Chemical Society; vol. 75; (1953); p. 2166						

Study Reference:		U.S. EPA (U.S. Environmental Protection Agency). (2012). <a href="#">Estimation Programs Interface Suite™ for Microsoft® Windows</a> , v 4.11 [Computer Program]. Washington, DC. HERO ID:2347246				
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	Appropriateness	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
Test Reliability	Reliability / Unbiased (Method Objectivity)	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	Reliability / Analytical Method	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
Other	Databases	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	Models	High	The models in EPI Suite™ have defined endpoints. Chemical domain and performance statistics for each model are known, and unambiguous algorithms are available in the EPI Suite™ documentation and/or cited references to establish their scientific validity. Many EPI Suite™ models have correlation coefficients >0.7, cross-validated correlation coefficients >0.5, and standard error values <0.3; however, correlation coefficients (r <sup>2</sup> , q <sup>2</sup> ) for the regressions of some environmental fate models (i.e., BIOWIN) are lower, as expected, compared to regressions which have specific experimental values such as water solubility or log Kow (octanol-water partition coefficient).	1	1	1
<b>Sum of scores:</b>				1	1	1
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1	<b>Overall Score (Rounded):</b>	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

## Tetramethyldisiloxanediol (CASRN 1118-15-6) Data Extraction Tables

Table 1. Physical State Study Summary

Study Type	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	3 values reported in Reaxys: 2 values were monoclinic crystal system (solid), 1 value was needle crystal shape (solid)		<a href="#">(Elsevier, 2021d)</a>	High

Table 2. Physical Properties Study Summary

Study Type	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	1 property reported in Reaxys: color – white		<a href="#">(Elsevier, 2021d)</a>	High

Table 3. Melting Point Study Summary

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	62–68 °C	19 values were reported in Reaxys; 8 values were in the range of 62–68 °C; one value was outside of this range; 9 values were reported with the test substance in a solvent.	<a href="#">(Elsevier, 2021d)</a>	High
Experimental	NR	66 °C	NR	<a href="#">(Haynes, 2014)</a>	High

Table 4. Boiling Point Study Summary

No Boiling Point data were identified for this chemical.



Table 5. Density Study Summary

Study Type	Study Details	Reference Substance	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental				1.08–1.15 g/cm <sup>3</sup>	4 values reported in Reaxys; 2 values were 1.118 g/cm <sup>3</sup> at 16 °C; 2 values did not have measurement temperatures. Crystallographic density.	( <a href="#">Elsevier, 2021d</a> )	High
Experimental				1.095 g/cm <sup>3</sup>	density at 25 °C	( <a href="#">Haynes, 2014</a> )	High

Table 6. Vapor Pressure Study Summary

No Vapor Pressure data were identified for this chemical.

Table 7. Vapor Density Study Summary

No Vapor Density data were identified for this chemical.

Table 8. Water Solubility Study Summary

Study Type	Substance Purity	Temperature	pH	Analytical Method	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	20–25 °C	NR		110–115 g/L	3 values reported in Reaxys, reported as 100 g solvent (water) dissolves 11–11.5 g substance	( <a href="#">Elsevier, 2021d</a> )	High
Experimental	NR	NR	NR		0.662 M	Equivalent to 110,000 mg/L based on MW 166.32 g/mol	( <a href="#">U.S. EPA, 2021a</a> )	High
Experimental	NR	NR	NR		0.661 M	Equivalent to 110,000 mg/L based on MW 166.32 g/mol	( <a href="#">U.S. EPA, 2021a</a> )	High
Experimental	NR	NR	NR		0.66 M	Equivalent to 100,000 mg/L based on MW 166.32 g/mol	( <a href="#">NLM, 2021a</a> )	High

#### Table 9. Octanol Water Coefficient (logKow) Study Summary

No Octanol Water Coefficient (logKow) data were identified for this chemical.

#### Table 10. Henry's Law Constant Study Summary

No Henry's Law data were identified for this chemical.

#### Table 11. Flash Point Study Summary

No Flash Point data were identified for this chemical.

#### Table 12. Auto Flammability Study Summary

No Autoflammability data were identified for this chemical.

#### Table 13. Viscosity Study Summary

No Viscosity data were identified for this chemical.

#### Table 14. Refractive Index Study Summary

Study Type	Apparatus	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	25 °C	1.457–1.466	2 values reported in Reaxys: 1.457–1.461 (n1) and 1.462–1.466 (n2), 589.3 nm	<a href="#">(Elsevier, 2021d)</a>	High

#### Table 15. Dielectric Constant Study Summary

No Dielectric Constant data were identified for this chemical.

EPI Suite™ Model Outputs  
(U.S. EPA, 2012)

SMILES: [Si](O)(O[Si](O)(C)C)(C)C  
CHEM: 1,3-Disiloxanediol, 1,1,3,3-tetramethyl-  
MOL FOR: C4 H14 O3 Si2  
MOL WT: 166.33

----- EPI SUMMARY (v4.11) -----

Physical Property Inputs:

Log Kow (octanol-water): -----  
Boiling Point (°C): -----  
Melting Point (°C): 66.00  
Vapor Pressure (mm Hg): -----  
Water Solubility (mg/L): 1.1E+005  
Henry LC (atm-m3/mole): -----

Log Octanol-Water Partition Coef (SRC):  
Log Kow (KOWWIN v1.68 estimate) = 1.74

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (°C): 236.15 (Adapted Stein & Brown method)  
Melting Pt (°C): 13.78 (Mean or Weighted MP)  
VP(mm Hg, 25 °C): 0.00196 (Modified Grain method)  
VP (Pa, 25 °C): 0.261 (Modified Grain method)  
Subcooled liquid VP: 0.00474 mm Hg (25 °C, Mod-Grain method): 0.632 Pa (25 °C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):

Water Solubility at 25 °C (mg/L): 914.6  
log Kow used: 1.74 (estimated)  
melt pt used: 66.00 °C  
Water Sol (Exper. database match) = 1.1E+005 mg/L (25 °C)  
Exper. Ref: BEILSTEIN

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 1.5402E+005 mg/L

ECOSAR Class Program (ECOSAR v1.11):

Class(es) found:  
Neutral Organics

Henrys Law Constant (25 °C) [HENRYWIN v3.20]:

Bond Method: 1.59E-008 atm-m3/mole (1.61E-003 Pa-m3/mole)  
Group Method: Incomplete  
For Henry LC Comparison Purposes:  
User-Entered Henry LC: not entered  
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:  
HLC: 3.900E-009 atm-m3/mole (3.951E-004 Pa-m3/mole)  
VP: 0.00196 mm Hg (source: MPBPVP)

WS: 1.1E+005 mg/L (source: User-Entered)

Log Octanol-Air Partition Coefficient (25 °C) [KOAWIN v1.10]:

Log Kow used: 1.74 (KowWin est)

Log Kaw used: -6.187 (HenryWin est)

Log Koa (KOAWIN v1.10 estimate): 7.927

Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model): 0.6684

Biowin2 (Non-Linear Model): 0.6563

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.8316 (weeks)

Biowin4 (Primary Survey Model): 3.6078 (days-weeks)

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model): 0.2190

Biowin6 (MITI Non-Linear Model): 0.0999

Anaerobic Biodegradation Probability:

Biowin7 (Anaerobic Linear Model): 0.5178

Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):

Structure incompatible with current estimation method!

Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 0.632 Pa (0.00474 mm Hg)

Log Koa (Koawin est): 7.927

Kp (particle/gas partition coef. (m<sup>3</sup>/ug)):

Mackay model: 4.75E-006

Octanol/air (Koa) model: 2.07E-005

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model: 0.000171

Mackay model: 0.00038

Octanol/air (Koa) model: 0.00166

Atmospheric Oxidation (25 °C) [AopWin v1.92]:

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 7.4984 E-12 cm<sup>3</sup>/molecule-sec

Half-Life = 1.426 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)

Half-Life = 17.117 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

0.000276 (Junge-Pankow, Mackay avg)

0.00166 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc: 340.7 L/kg (MCI method)

Log Koc: 2.532 (MCI method)  
Koc: 32.34 L/kg (Kow method)  
Log Koc: 1.510 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 °C) [HYDROWIN v2.00]:  
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):  
Log BCF from regression-based method = 0.817 (BCF = 6.562 L/kg wet-wt)  
Log Biotransformation Half-life (HL) = -0.4475 days (HL = 0.3569 days)  
Log BCF Arnot-Gobas method (upper trophic) = 0.795 (BCF = 6.23)  
Log BAF Arnot-Gobas method (upper trophic) = 0.795 (BAF = 6.23)  
log Kow used: 1.74 (estimated)

Volatilization from Water:  
Henry LC: 1.59E-008 atm-m<sup>3</sup>/mole (estimated by Bond SAR Method)  
Half-Life from Model River: 4.749E+004 hours (1979 days)  
Half-Life from Model Lake: 5.182E+005 hours (2.159E+004 days)

Removal in Wastewater Treatment:  
Total removal 2.07 percent  
Total biodegradation: 0.09 percent  
Total sludge adsorption: 1.97 percent  
Total to Air: 0.00 percent  
(using 10000 hr Bio P,A,S)

Level III Fugacity Model:  
Mass Amount Half-Life Emissions  
(percent) (hr) (kg/hr)

Air	0.246	34.2	1000
Water	17.9	360	1000
Soil	81.6	720	1000
Sediment	0.258	3.24E+003	0

Persistence Time: 722 hr

## Data Evaluation Tables

<b>Study Reference:</b>		<b>Elsevier (2021). Reaxys: physical-chemical property data for tetramethyl-1,3-disiloxanediol. CAS Registry Number: 1118-15-6. HERO ID: 7994661</b>				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated NR)</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	<b>Reliability / Analytical Method</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				2	2	2
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1	<b>Overall Score (Rounded):</b>	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Physical State reported by this reference. Cited references: Hyde 1953; Kakudo et al. 1953; Kakudo et al 1953.						

<b>Study Reference:</b> Elsevier (2021). Reaxys: physical-chemical property data for tetramethyl-1,3-disiloxanediol. CAS Registry Number: 1118-15-6. HERO ID: 7994661						
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	<b>Reliability / Analytical Method</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				2	2	2
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1	<b>Overall Score (Rounded):</b>	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Physical Properties reported by this reference.  
Cited reference: Lucas; Martin; Journal of the American Chemical Society; vol. 74; (1952); p. 5225, View in Reaxys

<b>Study Reference:</b>		<b>Elsevier (2021). Reaxys: physical-chemical property data for tetramethyl-1,3-disiloxanediol. CAS Registry Number: 1118-15-6. HERO ID: 7994661</b>				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference.  
Cited references: Makarova et al. 2006; Lucas 1952; Cella et al. 1994; Cypryk et al. 1993; Lickiss et al. 1993; Zachernyuk et al. 1985; Lebedev et al. 1979; Martyakova et al. 1976; Baratova et al. 1975; Andrianov 1974; Ungurenasu 1961; Borisov et al. 1966; Barnes 1966.



<b>Study Reference:</b>		<b>Haynes, W. M. (2014). CRC Handbook of Chemistry and Physics 1,1,3,3-Tetramethyl-1,3-disiloxanediol. Boca Raton, FL, CRC Press. Taylor &amp; Francis Group. HERO ID: 7998725</b>				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference.

<b>Study Reference:</b>		<b>Elsevier (2021). Reaxys: physical-chemical property data for tetramethyl-1,3-disiloxanediol. CAS Registry Number: 1118-15-6. HERO ID: 7994661</b>				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/ repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				6	4	6
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.5	<b>Overall Score (Rounded):</b>	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Density reported by this reference.  
Cited references: Lickiss et al. 1993; Hyde 1953; Kakudo et al. 1953; Kakudo et al 1953.

<b>Study Reference:</b>		<b>Haynes, W. M. (2014). CRC Handbook of Chemistry and Physics 1,1,3,3-Tetramethyl-1,3-disiloxanediol. Boca Raton, FL, CRC Press. Taylor &amp; Francis Group. HERO ID: 7998725</b>				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/ repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				6	4	6
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.5	<b>Overall Score (Rounded):</b>	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Density reported by this reference.						

Study Reference: Elsevier (2021). Reaxys: physical-chemical property data for tetramethyl-1,3-disiloxanediol. CAS Registry Number: 1118-15-6. HERO ID: 7994661						
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	Reliability / Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Water Solubility reported by this reference.  
Cited references: Sokolow 1959; Hyde 1953; Hyde 1953

Study Reference:	U.S. EPA (2021). Chemistry dashboard information for 1,3-Disiloxanediol, 1,1,3,3- tetramethyl-. CAS registry number: 1118-15-6. HERO ID: 7995923					
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	Reliability / Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Water Solubility reported by this reference. Cited reference: Kovdienko, et. al. Molecular informatics 29.5 (2010): 394–406.						

<b>Study Reference:</b>		<b>U.S. EPA (2021). Chemistry dashboard information for 1,3-Disiloxanediol, 1,1,3,3- tetramethyl-. CAS registry number: 1118-15-6. HERO ID: 7995923</b>				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated NR)</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Water Solubility reported by this reference.  
Cited reference: PhysProp

<b>Study Reference:</b>		<b>NLM (2021). Pubchem: 1,3-Disiloxanediol, 1,1,3,3-tetramethyl-. CAS registry number: 1118-15-6. HERO ID: 7997877</b>				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	Medium	Data is from a publicly available secondary source with references to non-peer reviewed original sources.	2	1	2
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				8	5	8
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.6	<b>Overall Score (Rounded):</b>	1.6
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Water Solubility reported by this reference.  
Cited reference: EPA DSSTox

<b>Study Reference:</b> Elsevier (2021). Reaxys: physical-chemical property data for tetramethyl-1,3-disiloxanediol. CAS Registry Number: 1118-15-6. HERO ID: 7994661						
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				6	4	6
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.5	<b>Overall Score (Rounded):</b>	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Refractive Index reported by this reference.  
Cited reference: Hyde; Journal of the American Chemical Society; vol. 75; (1953); p. 2166, View in Reaxys



Study Reference:		U.S. EPA (U.S. Environmental Protection Agency). (2012). <a href="#">Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11</a> [Computer Program]. Washington, DC. HERO ID:2347246				
Domain	Metric	Qualitative Determination ( <i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	Appropriateness	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
Test Reliability	Reliability / Unbiased (Method Objectivity)	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	Reliability / Analytical Method	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
Other	Databases	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	Models	High	The models in EPI Suite™ have defined endpoints. Chemical domain and performance statistics for each model are known, and unambiguous algorithms are available in the EPI Suite™ documentation and/or cited references to establish their scientific validity. Many EPI Suite™ models have correlation coefficients >0.7, cross-validated correlation coefficients >0.5, and standard error values <0.3; however, correlation coefficients (r <sup>2</sup> , q <sup>2</sup> ) for the regressions of some environmental fate models ( <i>i.e.</i> , BIOWIN) are lower, as expected, compared to regressions which have specific experimental values such as water solubility or log Kow (octanol-water partition coefficient).	1	1	1
<b>Sum of scores:</b>				1	1	1
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1	<b>Overall Score (Rounded):</b>	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

## Hexamethyltrisiloxanediol (CASRN 3663-50-1) Data Extraction Tables

Table 1. Physical State Study Summary

No Physical State data were identified for this chemical.

Table 2. Physical Properties Study Summary

No Physical Properties data were identified for this chemical.

Table 3. Melting Point Study Summary

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	-23 to -1.9 °C	2 values were reported in Reaxys.	<a href="#">(Elsevier, 2021a)</a>	High

Table 4. Boiling Point Study Summary

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	79–91 °C	5 values were reported in Reaxys; 3 were in the range of 79–91°C at 2–3 torr; the other two were 106 °C at 6 torr and 72–74°C at 0.3 torr	<a href="#">(Elsevier, 2021a)</a>	High

Table 5. Density Study Summary

Study Type	Study Details	Reference Substance	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental				0.991 to 1.0127 g/cm <sup>3</sup>	5 values were reported in Reaxys in the range of 0.991– 1.0127 g/cm <sup>3</sup> , at 20–25 °C (reference temperature 4 °C)	<a href="#">(Elsevier, 2021a)</a>	High

Table 6. Vapor Pressure Study Summary

No Vapor Pressure data were identified for this chemical.

Table 7. Vapor Density Study Summary

No Vapor Density data were identified for this chemical.

Table 8. Water Solubility Study Summary

No Water Solubility data were identified for this chemical.

#### Table 9. Octanol Water Coefficient (logKow) Study Summary

No Octanol Water Coefficient (logKow) data were identified for this chemical.

#### Table 10. Henry's Law Constant Study Summary

No Henrys Law data were identified for this chemical.

#### Table 11. Flash Point Study Summary

No Flash Point data were identified for this chemical.

#### Table 12. Auto Flammability Study Summary

No Autoflammability data were identified for this chemical.

#### Table 13. Viscosity Study Summary

No Viscosity data were identified for this chemical.

#### Table 14. Refractive Index Study Summary

Study Type	Apparatus	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	20–25 °C	1.405–1.409	6 values were reported in Reaxys in the range of 1.405–1.409, 589 nm	<a href="#">(Elsevier, 2021a)</a>	High

#### Table 15. Dielectric Constant Study Summary

No Dielectric Constant data were identified for this chemical.

EPI Suite™ Model Outputs  
([U.S. EPA, 2012](#))

SMILES: [Si](O)(O[Si](O[Si](O)(C)C)(C)C)(C)C  
CHEM: 1,5-Trisiloxanediol, 1,1,3,3,5,5-hexamethyl-  
MOL FOR: C6 H20 O4 Si3  
MOL WT: 240.48

----- EPI SUMMARY (v4.11) -----

Physical Property Inputs:

Log Kow (octanol-water): -----  
Boiling Point (°C): -----  
Melting Point (°C): -----  
Vapor Pressure (mm Hg): -----  
Water Solubility (mg/L): -----  
Henry LC (atm-m<sup>3</sup>/mole): -----

Log Octanol-Water Partition Coef (SRC):  
Log Kow (KOWWIN v1.68 estimate) = 3.20

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (°C): 276.03 (Adapted Stein & Brown method)  
Melting Pt (°C): 35.49 (Mean or Weighted MP)  
VP(mm Hg, 25 °C): 0.000289 (Modified Grain method)  
VP (Pa, 25 °C): 0.0385 (Modified Grain method)  
Subcooled liquid VP: 0.000359 mm Hg (25 °C, Mod-Grain method): 0.0478 Pa (25 °C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):

Water Solubility at 25 °C (mg/L): 20.67  
log Kow used: 3.20 (estimated)  
no-melting pt equation used

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 7163.9 mg/L

ECOSAR Class Program (ECOSAR v1.11):

Class(es) found:  
Neutral Organics

Henrys Law Constant (25 °C) [HENRYWIN v3.20]:

Bond Method: 2.18E-008 atm-m<sup>3</sup>/mole (2.21E-003 Pa-m<sup>3</sup>/mole)  
Group Method: Incomplete  
For Henry LC Comparison Purposes:  
User-Entered Henry LC: not entered  
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:  
HLC: 4.424E-006 atm-m<sup>3</sup>/mole (4.483E-001 Pa-m<sup>3</sup>/mole)  
VP: 0.000289 mm Hg (source: MPBPVP)  
WS: 20.7 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 °C) [KOAWIN v1.10]:  
Log Kow used: 3.20 (KowWin est)  
Log Kaw used: -6.050 (HenryWin est)  
Log Koa (KOAWIN v1.10 estimate): 9.250  
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):  
Biowin1 (Linear Model): 0.6331  
Biowin2 (Non-Linear Model): 0.3998  
Expert Survey Biodegradation Results:  
Biowin3 (Ultimate Survey Model): 2.6677 (weeks-months)  
Biowin4 (Primary Survey Model): 3.5008 (days-weeks)  
MITI Biodegradation Probability:  
Biowin5 (MITI Linear Model): -0.0008  
Biowin6 (MITI Non-Linear Model): 0.0134  
Anaerobic Biodegradation Probability:  
Biowin7 (Anaerobic Linear Model): 0.3587  
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):  
Structure incompatible with current estimation method!

Sorption to aerosols (25 °C)[AEROWIN v1.00]:  
Vapor pressure (liquid/subcooled): 0.0479 Pa (0.000359 mm Hg)  
Log Koa (Koawin est): 9.250  
Kp (particle/gas partition coef. (m<sup>3</sup>/ug)):  
Mackay model: 6.27E-005  
Octanol/air (Koa) model: 0.000437  
Fraction sorbed to airborne particulates (phi):  
Junge-Pankow model: 0.00226  
Mackay model: 0.00499  
Octanol/air (Koa) model: 0.0337

Atmospheric Oxidation (25 °C) [AopWin v1.92]:  
Hydroxyl Radicals Reaction:  
OVERALL OH Rate Constant = 7.7976 E-12 cm<sup>3</sup>/molecule-sec  
Half-Life = 1.372 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)  
Half-Life = 16.460 Hrs  
Ozone Reaction:  
No Ozone Reaction Estimation  
Fraction sorbed to airborne particulates (phi):  
0.00362 (Junge-Pankow, Mackay avg)  
0.0337 (Koa method)  
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):  
Koc: 2644 L/kg (MCI method)  
Log Koc: 3.422 (MCI method)  
Koc: 598.2 L/kg (Kow method)

Log Koc: 2.777 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 °C) [HYDROWIN v2.00]:  
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):

Log BCF from regression-based method = 1.777 (BCF = 59.85 L/kg wet-wt)

Log Biotransformation Half-life (HL) = 0.2998 days (HL = 1.994 days)

Log BCF Arnot-Gobas method (upper trophic) = 2.145 (BCF = 139.7)

Log BAF Arnot-Gobas method (upper trophic) = 2.145 (BAF = 139.7)

log Kow used: 3.20 (estimated)

Volatilization from Water:

Henry LC: 2.18E-008 atm-m<sup>3</sup>/mole (estimated by Bond SAR Method)

Half-Life from Model River: 4.165E+004 hours (1735 days)

Half-Life from Model Lake: 4.545E+005 hours (1.894E+004 days)

Removal in Wastewater Treatment:

Total removal 7.80 percent

Total biodegradation: 0.14 percent

Total sludge adsorption: 7.66 percent

Total to Air: 0.00 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)	
Air	0.134	32.9	1000
Water	12	900	1000
Soil	86	1.8E+003	1000
Sediment	1.81	8.1E+003	0

Persistence Time: 1.7E+003 hr

## Data Evaluation Tables

Study Reference: Elsevier (2021). Reaxys: physical-chemical property data for 1,1,3,3,5,5- hexamethyltrisiloxane-1,5-diol. CAS Registry Number: 3663-50-1. HERO ID: 7992314						
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated NR)	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/ chemical properties or behaviors.	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	Reliability / Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference.  
Cited reference: Patent; Union Carbide; FR1399256; (1965); (A); Chem.Abstr.; vol. 63; nb. 16383e; (1965); Chem.Abstr.; vol. 63; nb. 16383e; (1965); Sokolow; Zhurnal Obschei Khimii; vol. 29; (1959); p. 258,261, 263; engl. Ausg. S. 262, 265, 266.

<b>Study Reference:</b> Elsevier (2021). Reaxys: physical-chemical property data for 1,1,3,3,5,5- hexamethyltrisiloxane-1,5-diol. CAS Registry Number: 3663-50-1. HERO ID: 7992314						
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated NR)</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Boiling Point reported by this reference.  
Cited references: Zachernyuk et al. 1985; Kaufman et al. 1970; Union Carbide Patent 1965; Harris 1963; Andrianov et al. 1962



<b>Study Reference:</b>		Elsevier (2021). Reaxys: physical-chemical property data for 1,1,3,3,5,5- hexamethyltrisiloxane-1,5-diol. CAS Registry Number: 3663-50-1. HERO ID: 7992314				
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated NR)</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				6	4	6
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.5	<b>Overall Score (Rounded):</b>	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Density reported by this reference.  
Cited references: Voronkov et al. 1970; Kaufman and Karlin 1970; Union Carbide Patent 1965; Andrianov et al. 1962; Sokolow 1959.

<b>Study Reference:</b> Elsevier (2021). Reaxys: physical-chemical property data for 1,1,3,3,5,5- hexamethyltrisiloxane-1,5-diol. CAS Registry Number: 3663-50-1. HERO ID: 7992314						
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated NR)</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				6	4	6
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.5	<b>Overall Score (Rounded):</b>	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Refractive Index reported by this reference. Cited references: Voronokov et al. 1971; Kaufman and Karlin 1970; Union Carbide Patent 1965; Harris 1963; Andrianov 1962; Sokolow 1959.						

Study Reference: U.S. EPA (U.S. Environmental Protection Agency). (2012). <a href="#">Estimation Programs Interface Suite™ for Microsoft® Windows, v 4.11</a> [Computer Program]. Washington, DC. HERO ID:2347246						
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	Appropriateness	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
Test Reliability	Reliability / Unbiased (Method Objectivity)	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	Reliability / Analytical Method	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
Other	Databases	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	Models	High	The models in EPI Suite™ have defined endpoints. Chemical domain and performance statistics for each model are known, and unambiguous algorithms are available in the EPI Suite™ documentation and/or cited references to establish their scientific validity. Many EPI Suite™ models have correlation coefficients >0.7, cross-validated correlation coefficients >0.5, and standard error values <0.3; however, correlation coefficients (r <sup>2</sup> , q <sup>2</sup> ) for the regressions of some environmental fate models (i.e., BIOWIN) are lower, as expected, compared to regressions which have specific experimental values such as water solubility or log Kow (octanol-water partition coefficient).	1	1	1
<b>Sum of scores:</b>				1	1	1
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1	<b>Overall Score (Rounded):</b>	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

## Octamethyltetrasiloxanediol (CASRN 3081-07-0) Data Extraction Tables

Table 1. Physical State Study Summary

No Physical State data were identified for this chemical.

Table 2. Physical Properties Study Summary

No Physical Properties data were identified for this chemical.

Table 3. Melting Point Study Summary

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	-5 °C	NR	( <a href="#">Elsevier, 2021b</a> )	High

Table 4. Boiling Point Study Summary

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	97–100 °C	1 value reported in Reaxys at 2 torr	( <a href="#">Elsevier, 2021b</a> )	High
Experimental	NR	86–88 °C	1 value reported in Reaxys at 0.4 torr	( <a href="#">Elsevier, 2021b</a> )	High

Table 5. Density Study Summary

Study Type	Study Details	Reference Substance	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental				0.9881–0.9886 g/cm <sup>3</sup>	2 values reported in Reaxys; reference temperature 4 °C, measurement temperature 20 °C	( <a href="#">Elsevier, 2021b</a> )	High

Table 6. Vapor Pressure Study Summary

No Vapor Pressure data were identified for this chemical.

Table 7. Vapor Density Study Summary

No Vapor Density data were identified for this chemical.

#### Table 8. Water Solubility Study Summary

No Water Solubility data were identified for this chemical.

#### Table 9. Octanol Water Coefficient (logKow) Study Summary

No Octanol Water Coefficient (logKow) data were identified for this chemical.

#### Table 10. Henry's Law Constant Study Summary

No Henry's Law data were identified for this chemical.

#### Table 11. Flash Point Study Summary

No Flash Point data were identified for this chemical.

#### Table 12. Auto Flammability Study Summary

No Autoflammability data were identified for this chemical.

#### Table 13. Viscosity Study Summary

No Viscosity data were identified for this chemical.

#### Table 14. Refractive Index Study Summary

Study Type	Apparatus	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	20–25 °C	1.4054–1.4088	3 values were reported in Reaxys, 589 nm	<a href="#">(Elsevier, 2021b)</a>	High

#### Table 15. Dielectric Constant Study Summary

No Dielectric Constant data were identified for this chemical.

EPI Suite™ Model Outputs  
(U.S. EPA, 2012)

SMILES: [Si](O)(O[Si](O[Si](O[Si](O)(C)C)(C)C)(C)C)(C)C  
CHEM: 1,7-Tetrasiloxanediol, 1,1,3,3,5,5,7,7-octamethyl-  
MOL FOR: C8 H26 O5 Si4  
MOL WT: 314.64

----- EPI SUMMARY (v4.11) -----

Physical Property Inputs:

Log Kow (octanol-water): -----  
Boiling Point (°C): -----  
Melting Point (°C): -----  
Vapor Pressure (mm Hg): -----  
Water Solubility (mg/L): -----  
Henry LC (atm-m<sup>3</sup>/mole): -----

Log Octanol-Water Partition Coef (SRC):  
Log Kow (KOWWIN v1.68 estimate) = 4.65

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):

Boiling Pt (°C): 306.15 (Adapted Stein & Brown method)  
Melting Pt (°C): 40.55 (Mean or Weighted MP)  
VP (mm Hg, 25 °C): 3.53E-005 (Modified Grain method)  
VP (Pa, 25 °C): 0.0047 (Modified Grain method)  
Subcooled liquid VP: 4.88E-005 mm Hg (25 °C, Mod-Grain method)  
: 0.0065 Pa (25 °C, Mod-Grain method)

Water Solubility Estimate from Log Kow (WSKOW v1.42):

Water Solubility at 25 °C (mg/L): 3.017  
log Kow used: 4.65 (estimated)  
no-melting pt equation used

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 301.53 mg/L

ECOSAR Class Program (ECOSAR v1.11):

Class(es) found:  
Neutral Organics

Henrys Law Constant (25 °C) [HENRYWIN v3.20]:

Bond Method: 3.00E-008 atm-m<sup>3</sup>/mole (3.04E-003 Pa-m<sup>3</sup>/mole)  
Group Method: Incomplete  
For Henry LC Comparison Purposes:  
User-Entered Henry LC: not entered  
Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:  
HLC: 4.844E-006 atm-m<sup>3</sup>/mole (4.908E-001 Pa-m<sup>3</sup>/mole)  
VP: 3.53E-005 mm Hg (source: MPBPVP)  
WS: 3.02 mg/L (source: WSKOWWIN)

Log Octanol-Air Partition Coefficient (25 °C) [KOAWIN v1.10]:  
Log Kow used: 4.65 (KowWin est)  
Log Kaw used: -5.911 (HenryWin est)  
Log Koa (KOAWIN v1.10 estimate): 10.561  
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):  
Biowin1 (Linear Model): 0.5978  
Biowin2 (Non-Linear Model): 0.1886  
Expert Survey Biodegradation Results:  
Biowin3 (Ultimate Survey Model): 2.5039 (weeks-months)  
Biowin4 (Primary Survey Model): 3.3938 (days-weeks)  
MITI Biodegradation Probability:  
Biowin5 (MITI Linear Model): -0.2206  
Biowin6 (MITI Non-Linear Model): 0.0017  
Anaerobic Biodegradation Probability:  
Biowin7 (Anaerobic Linear Model): 0.1995  
Ready Biodegradability Prediction: NO

Hydrocarbon Biodegradation (BioHCwin v1.01):  
Structure incompatible with current estimation method!

Sorption to aerosols (25 °C)[AEROWIN v1.00]:  
Vapor pressure (liquid/subcooled): 0.00651 Pa (4.88E-005 mm Hg)  
Log Koa (Koawin est): 10.561  
Kp (particle/gas partition coef. (m<sup>3</sup>/ug)):  
Mackay model: 0.000461  
Octanol/air (Koa) model: 0.00893  
Fraction sorbed to airborne particulates (phi):  
Junge-Pankow model: 0.0164  
Mackay model: 0.0356  
Octanol/air (Koa) model: 0.417

Atmospheric Oxidation (25 °C) [AopWin v1.92]:  
Hydroxyl Radicals Reaction:  
OVERALL OH Rate Constant = 8.0968 E-12 cm<sup>3</sup>/molecule-sec  
Half-Life = 1.321 Days (12-hr day; 1.5E6 OH/cm<sup>3</sup>)  
Half-Life = 15.852 Hrs  
Ozone Reaction:  
No Ozone Reaction Estimation  
Fraction sorbed to airborne particulates (phi):  
0.026 (Junge-Pankow, Mackay avg)  
0.417 (Koa method)  
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):  
Koc: 2.052E+004 L/kg (MCI method)  
Log Koc: 4.312 (MCI method)  
Koc: 1.085E+004 L/kg (Kow method)

Log Koc: 4.035 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 °C) [HYDROWIN v2.00]:  
Rate constants can NOT be estimated for this structure!

Bioaccumulation Estimates (BCFBAF v3.01):

Log BCF from regression-based method = 2.737 (BCF = 545.8 L/kg wet-wt)

Log Biotransformation Half-life (HL) = 1.0470 days (HL = 11.14 days)

Log BCF Arnot-Gobas method (upper trophic) = 3.344 (BCF = 2208)

Log BAF Arnot-Gobas method (upper trophic) = 3.425 (BAF = 2661)

log Kow used: 4.65 (estimated)

Volatilization from Water:

Henry LC: 3E-008 atm-m<sup>3</sup>/mole (estimated by Bond SAR Method)

Half-Life from Model River: 3.462E+004 hours (1442 days)

Half-Life from Model Lake: 3.778E+005 hours (1.574E+004 days)

Removal in Wastewater Treatment:

Total removal: 63.62 percent

Total biodegradation: 0.58 percent

Total sludge adsorption: 63.05 percent

Total to Air: 0.00 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount Half-Life Emissions

(percent)	(hr)	(kg/hr)	
Air	0.157	31.7	1000
Water	0.3	900	1000
Soil	77.5	1.8E+003	1000
Sediment	12.1	8.1E+003	0

Persistence Time: 1.84E+003 hr



## Data Evaluation Tables

Study Reference: Elsevier (2021). Reaxys: physical-chemical property data for 1,1,3,3,5,5,7,7- octamethyltetrasiloxane-1,7-diol. CAS Registry Number: 3081-07-0. HERO ID: 7991715						
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	Reliability / Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference.  
Cited reference: Zhurnal Obshchei Khimii; vol. 29; (1959); p. 258,261, 263; engl. Ausg. S. 262, 265, 266,

<b>Study Reference:</b> Elsevier (2021). Reaxys: physical-chemical property data for 1,1,3,3,5,5,7,7- octamethyltetrasiloxane-1,7-diol. CAS Registry Number: 3081-07-0. HERO ID: 7991715						
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties or behaviors.	1	1	1
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Boiling Point reported by this reference.  
Cited reference: Andrianov, K.A. et al.; Bulletin of the Academy of Sciences of the USSR Division of Chemical Science; (1962); p. 2144–2146; Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya; (1962); p. 2243–2245.

<b>Study Reference:</b> Elsevier (2021). Reaxys: physical-chemical property data for 1,1,3,3,5,5,7,7- octamethyltetrasiloxane-1,7-diol. CAS Registry Number: 3081-07-0. HERO ID: 7991715						
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/ chemical properties or behaviors.	1	1	1
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				7	5	7
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.4	<b>Overall Score (Rounded):</b>	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

The reviewer agreed with the overall rating for the Boiling Point reported by this reference.  
Cited reference: Harris; Journal of the Chemical Society; (1963); p. 5978, 5981.

<b>Study Reference:</b> Elsevier (2021). Reaxys: physical-chemical property data for 1,1,3,3,5,5,7,7- octamethyltetrasiloxane-1,7-diol. CAS Registry Number: 3081-07-0. HERO ID: 7991715						
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated NR)</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	<b>Appropriateness</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	<b>Reliability / Analytical Method</b>	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
<b>Other</b>	<b>Databases</b>	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	<b>Models</b>	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				6	4	6
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.5	<b>Overall Score (Rounded):</b>	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
The reviewer agreed with the overall rating for the Density reported by this reference. Cited references: Andrianov, K.A. et al.; Bulletin of the Academy of Sciences of the USSR Division of Chemical Science; (1962); p. 2144–2146; Sokolow; Zhurnal Obshchei Khimii; vol. 29; (1959); p. 258,261, 263; engl. Ausg. S. 262, 265, 266						

Study Reference:	Elsevier (2021). Reaxys: physical-chemical property data for 1,1,3,3,5,5,7,7- octamethyltetrasiloxane-1,7-diol. CAS Registry Number: 3081-07-0. HERO ID: 7991715					
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
	Reliability / Analytical Method	Medium	The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
<b>Sum of scores:</b>				6	4	6
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1.5	<b>Overall Score (Rounded):</b>	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High
<p>The reviewer agreed with the overall rating for the Refractive Index reported by this reference.  Cited references: Harris 1963; Andrianov,K.A. et al.; Bulletin of the Academy of Sciences of the USSR Division of Chemical Science; (1962); p. 2144 - 2146; Sokolow; Zhurnal Obshechi Khimii; vol. 29; (1959); p. 258,261, 263; engl. Ausg. S. 262, 265, 266</p>						

<b>Study Reference:</b> U.S. EPA (U.S. Environmental Protection Agency). (2012). <a href="#">Estimation Programs Interface Suite™</a> for Microsoft® Windows, v 4.11 [Computer Program]. Washington, DC. HERO ID:2347246						
<b>Domain</b>	<b>Metric</b>	<b>Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])</b>	<b>Comments</b>	<b>Metric Score</b>	<b>Metric Weighting Factor</b>	<b>Weighted Score</b>
<b>Substance</b>	<b>Representativeness</b>	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	<b>Appropriateness</b>	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
<b>Test Reliability</b>	<b>Reliability / Unbiased (Method Objectivity)</b>	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	<b>Reliability / Analytical Method</b>	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
<b>Other</b>	<b>Databases</b>	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	<b>Models</b>	High	The models in EPI Suite™ have defined endpoints. Chemical domain and performance statistics for each model are known, and unambiguous algorithms are available in the EPI Suite™ documentation and/or cited references to establish their scientific validity. Many EPI Suite™ models have correlation coefficients >0.7, cross-validated correlation coefficients >0.5, and standard error values <0.3; however, correlation coefficients (r <sup>2</sup> , q <sup>2</sup> ) for the regressions of some environmental fate models (i.e., BOWIN) are lower, as expected, compared to regressions which have specific experimental values such as water solubility or log Kow (octanol-water partition coefficient).	1	1	1
<b>Sum of scores:</b>				1	1	1
High	Medium	Low	<b>Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:</b>	1	<b>Overall Score (Rounded):</b>	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			<b>Overall Quality Level:</b>	High

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