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

Supplemental File:

Data Extraction and Data Evaluation Tables for Physical and Chemical Property Studies CASRN: 556-67-2

$$H_3C$$
 Si
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Data Extraction Tables

In each table, the value preliminarily selected for use in the risk evaluation is in bold.

Table 1. Physical State Study Summary for Octamethylcyclotetra- siloxane (D4)

Study Type	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	Oily liquid		(<u>O'Neil, 2013</u>)	High
Experimental	Colorless liquid		(<u>RSC, 2020</u>)	High
Experimental	Oily liquid		(NLM, 2020)	High
Experimental	Smooth, viscous liquid		(<u>NLM, 2020</u>)	High

Table 2. Physical Properties Study Summary for D4

Study Type	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	Colorless liquid		(<u>RSC, 2020</u>)	High
Experimental	Oily liquid		(<u>O'Neil, 2013</u>)	High
Experimental	Dry powder; liquid		(NLM, 2020)	Unacceptable
Experimental	Colorless, oily liquid		(NLM, 2020)	High
Experimental	D4 does not have an odor; qualitative description that was not the focus of the primary source		(<u>Fuller et al., 2020</u>)	Medium

Table 3. Melting Point Study Summary for D4

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	17.5–18.0 °C	17.6 °C average of 6 values	(<u>U.S. EPA, 2020</u>)	High
Experimental	NR	17.5 °C		(O"Neil, 2013)	High
Experimental	NR	17–18.5 °C	15 values were reported in Reaxys; 14 values were in the range of 17–18.5 °C; 1 value was outside this range.	(Elsevier, 2019)	High
Experimental	NR	17.10 °C		(<u>Haynes, 2014</u>)	High
Experimental	NR	17.5 °C		(<u>NLM, 2020</u>)	High
Experimental	NR	17.5 °C		(<u>RSC</u> , 2020)	High
Experimental	NR	17.5–18 °C		(<u>RSC</u> , 2020)	High
Experimental	NR	17–18 °C		(<u>RSC</u> , 2020)	High
Experimental	NR	17–18 °C		(<u>RSC</u> , 2020)	High
Experimental	NR	17–18 °C		(<u>RSC</u> , 2020)	High
Experimental	NR	17–18 °C		(<u>RSC, 2020</u>)	High
Experimental	NR	17–18 °C		(<u>RSC, 2020</u>)	High
Experimental; differential scanning calorimeters ("DSC Q100")	>99.8%	291.12 K	Experimental vapor pressures at 312.97–450.42 K also reported in this study.	(Abbas et al., 2011)	High

Table 4. Boiling Point Study Summary for D4

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	176 °C	176 °C average of 4 values	(<u>U.S. EPA, 2020</u>)	High
Experimental	NR	175 °C	STP	(O'Neil, 2013)	High
Experimental	NR	74 °C	20 mm Hg	(<u>O'Neil, 2013</u>)	High
Experimental	NR	170–176.4 °C	750–760 torr; 28 values were reported in Reaxys; 19 of these values were reported in the range of 170–176.4 °C at 750–760 torr; 9 values were outside this range or measured at unreported or non-standard pressures.	(<u>Elsevier, 2019</u>)	High
Experimental	NR	175.4 °C		(<u>Haynes, 2014</u>)	High
Experimental	NR	175.8 °C		(NLM, 2020)	High
Experimental	NR	74 °C	20 mm Hg	(NLM, 2020)	High
Experimental	NR	175 °C		(<u>NLM, 2020</u>)	High
Experimental	NR	176 °C		(<u>RSC</u> , 2020)	High
Experimental	NR	175–176 °C		(<u>RSC</u> , 2020)	High
Experimental	NR	175–176 °C		(<u>RSC, 2020</u>)	High
Experimental	NR	175–176 °C		(<u>RSC, 2020</u>)	High
Experimental	NR	175–176 °C		(<u>RSC, 2020</u>)	High
Experimental	NR	175–176 °C		(<u>RSC, 2020</u>)	High

Table 5. Density Study Summary for D4

Study Type	Study Details	Reference Substance	Temperatu re	Result (g/cm ³)	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental				0.9558	Units not given	(O'Neil, 2013)	High
Experimental			19.99–25°C	0.9497– 0.9568	47 values were reported in Reaxys; 21 values were reported in the range of 0.9497–0.9568 g/cm³ at 19.99-25 °C; 26 values were outside this range or measured at unreported or non-standard temperatures.	(Elsevier, 2019)	High
Experimental			20 °C	0.9561		(<u>Haynes</u> , 2014)	High
Experimental				0.96	Relative density: water = 1	(<u>NLM, 2020</u>)	High
Experimental				0.9558	Units not given	(<u>NLM, 2020</u>)	High
Experimental				0.956	Reported as 0.956 g/mL	(<u>RSC, 2020</u>)	High
Experimental				0.956	Reported as 0.956 g/mL	(<u>RSC</u> , 2020)	High
Experimental				0.956	Reported as 0.956 g/mL	(<u>RSC</u> , 2020)	High
Experimental				0.956	Reported as 0.956 g/mL	(<u>RSC</u> , 2020)	High
Experimental			292.00 K	0.95755	Reported as 957.55 kg/m³ at 292.00 K; 957.55–790.24 kg/m³ at 292.00–433.15 K	(Palczewska- Tulinska and Oracz, 2005)	High
Experimental			293.15 K	0.95603	Reported as 0.95603 g/cm ³ measured at 293.15 K and atmospheric pressure, 102.355 ± 0.020 kPa	(Zhang et al., 2015)	High

Table 6. Vapor Pressure Study Summary for D4

Study Type	Substance Purity	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	NR	1.05 torr	Reported as 1.05 mm Hg	(<u>U.S. EPA,</u> 2020)	High
Experimental	NR	25 °C	1.05 torr	Reported as 1.05 mm Hg	(<u>NLM,</u> 2020)	High
Experimental	NR	21.7 °C	133.3 Pa		(<u>NLM,</u> 2020)	High
Experimental	NR	298.15 K	92.8–24.5 Pa	Gas chromatographic retention time (GCRT) technique P(GC) and Liquid state vapor pressure P(L). $P(GC) = 92.8 \pm 0.9 Pa$; $P(L) 124.5 \pm 6.2 Pa$ at 298.15 K. Std. dev. $P(L) \pm 6.2 Pa$; $P(GC) \pm 0.9$. Temperature ranges of retention time measurements 308.15-368.15 K.	(<u>Lei et al.,</u> 2010)	High
Experimental	NR	361.71– 459.65 K	≥5.36 to ≤ 133.26 kPa	Non-guideline; vapor pressures measured in an ebulliometer over the pressure range of 7–133 kPa; experimental data fit for Antoine equation and constants A, B, and C. Temperature measurement readings to the nearest 0.01K	(<u>Flaningam,</u> 1986)	Medium

Table 7. Vapor Density Study Summary for D4

No Vapor Density data was identified for this chemical.

Table 8. Water Solubility Study Summary for D4

Study Type	Substance Purity	Temperature	pН	Analytical Method	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	NR	NR		0.005 mg/L	Average of 2 values; 1.69E- 8 to 1.70E-8 mol/L	(U.S. EPA, 2020)	High
Experimental	NR	23 °C	NR			Reported as 189.86E6 mmol/L	(<u>Elsevier</u> , 2019)	Unacceptable
Experimental	NR	23°C	NR		0.056 mg/L		(NLM, 2020)	High
Experimental	NR	25 °C	NR		0.033 mg/L	Measured in synthetic seawater	(NLM, 2020)	High
Experimental	NR	NR	NR			Reported as "none"	(NLM, 2020)	Unacceptable
Experimental; non-turbulent method	NR	23 °C	NR	GC-MS	0.056 ppm	Reported as 56.0 ppb; also, aqueous solubility = 189.86 nmol/L	(<u>Varaprath et al., 1996</u>)	High
Experimental; Column generator	>99%	NR	NR		0.074 mg/L	Reported as 74 µg/L in freshwater	(<u>Sousa et al.,</u> 1995)	High
Experimental; Column generator	>99%	NR	NR		0.033 mg/L	Reported as 33 µg/L in saltwater	(Sousa et al., 1995)	High
Experimental	99.3%	40 °C	NR	GC-MS	0.161 mg/L	Reported as 544 nmol/L	(<u>Gee, 2015</u>)	High
Experimental	99.3%	60 °C	NR	GC-MS	0.4 mg/L	Reported as 1348 nmol/L	(<u>Gee, 2015</u>)	High
Experimental; Generator Column Method Following TSCA Test Standard 796.1860 and amendment #1	99%	25 °C	NR		29–38 μg/L	Mean is 33 μg/L for 7 measurements; Mean recovery from fresh and filtered seawater was 96.5±3.99% and 97.3±12.2%; RSD was 8.8 and 1.1% at 5.00 and 20.0 μg/L, respectively.	(Springborn Laboratories, 1989c)	High
Experimental; Generator Column Method Following TSCA Test Standard 796.1860 and amendment #1	99%	25 °C	NR		60–94 μg/L	Mean 74 μg/L for 12 measurements; Mean recovery 103+/-12.6%. Likely the same study as HERO ID 7006395	(Springborn Laboratories, 1989b)	High

Study Type	Substance Purity	Temperature	pН	Analytical Method	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	NR	NR		39–47 μg/L	Mean value 42+/-0.9 μg/L	(Bayer AG, 1990)	High
Experimental	NR	25 °C	NR		27–33 μg/L	Mean value 29.5 μg/L	(<u>Bayer AG,</u> 1990)	High
Experimental	NR	15–40 °C	NR		20–750 ppb	The large discrepancy between the results cannot be explained by either the duration of the 2 steps or the stirring temperature. Detection of microbubbles of D4 cannot be checked.	(Rhone-Poulenc Inc, 1990)	Medium
Experimental	NR	20 °C	NR		15–240 ppb	It is impossible to deduce a precise value from the present results.	(Rhone-Poulenc Inc, 1990)	Medium
Experimental	>99.5%	NR	NR		50 ppb	Water solubility determined as a result of log Kow measurement. First determination: 25 ppb in water; second determination: 53 ppb in water	(Dow Corning, 1987a)	High
Experimental	NR	NR	NR		40-80 ppb	Closed recirculating system: 76 ppb (unfiltered); 40 ppb (0.45-micron filter) Open recirculating system: 27 ± 3 ppb (possible evaporative loss) Separatory funnel: 8.1–2.9 ppm (unfiltered); 28–16 ppb (0.20–micron filter) D4 is not truly dispersed in water, may be present in various particle sizes.	(Dow Corning, 1987b)	High
Experimental; Non-Turbulent Partitioning of D4	>99% Pure	23 °C	NR		56 ppb	WS ranged from 50–60 ppb	(<u>Dow Corning</u> , 1991)	High

Study Type	Substance Purity	Temperature	pН	Analytical Method	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental; Generator Column Method Following TSCA Test Standard 796.1860 and amendment #1	99%	25 °C	NR		74 μg/L	Likely the same study as HERO ID 5889414	(Springborn Laboratories, 1989a)	High

Table 9. Octanol Water Coefficient (logKow) Study Summary for D4

Study Type	Substance Purity	Temperature	pН	Other Study Details (Amounts of substance liquid phases)	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	NR	NR	NR	6.74		(<u>U.S. EPA,</u> 2020)	High
Experimental	NR	21.6–21.7 °C	NR	NR	6.98	4 data points were reported in Reaxys; 2 of these values were reported as 6.98 at 21.6–21.7°C; 2 data points were measured at unreported temperatures.	(<u>Elsevier,</u> 2019)	High
Experimental	NR	NR	NR	NR	6.74	Average of three measurements	(<u>NLM,</u> 2020)	High
Experimental; double-syringe method	>98%	5.7; 12.2; 21.7; 34.8 °C	NR	2 air-tight syringes with an air sampling port and a water sampling port; concentration in water (µg/L): 1.4–2.0; 0.9–1.3; 0.8–1.5; 1.9–4.0	6.59– 7.13	Temperature has substantial effects on measured partition coefficients; equilibrium at 6 hrs	(Xu and Kropscott, 2014)	High
Experimental; double- syringe apparatus	98.1%	21.6; 21.7 °C	NR	2 air-tight syringes with an air sampling port and a water sampling port; concentration in water (mg/L): 1.53E-3; 1.84E-4	6.98	Equilibrium reached at 20 hrs; cryogenic cold trap, dry ice acetone bath	(Xu and Kropscott, 2012)	High

Study Type	Substance Purity	Temperature	рН	Other Study Details (Amounts of substance liquid phases)	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental; Draft OECD Guideline - Slow Stir Method	99.77; 2 area percent purity	25.1°C	NR	Slow-Stirring Method Using Gas Chromatography and Mass Spectrometry	6.488	at equilibrium	(Kozerski and Shawl, 2007)	High
Experimental	>99%	NR	NR	OECD classical partitioning between 50 mL octanol and 250 mL water	4.0		(Dow Corning, 1982)	High
Experimental	>99.5%	NR	NR	100 μL (0.0956 g) D4 in 25 g (30.23 mL) octanol placed in a 250 mL Wheaton bottle with 150 mL distilled water. The bottle was capped, agitated for an hour on a Burrell wrist-action shaker, and allowed to settle overnight.	5.10		(Dow Corning, 1987a)	High

Table 10. Henry's Law Constant Study Summary for D4

Study Type	Substance Purity	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	NR	12.0 atm-m³/mol		(<u>U.S. EPA, 2020</u>)	High
Experimental	>98%	5.7±0.2, 12.2±0.1, 34.8±0.2 °C	1.79–3.09	log Kaw = 1.79±0.07, 2.17±0.08 and 3.09±0.14 at 5.7, 12.2 and 34.8 °C, respectively; log Kaw = 2.74 at 25 °C based on linear regression analysis of data.	(Xu, 2014, 2535012)	High
Experimental	NR	NR	12.00 atm-m ³ /mol		(<u>NLM, 2020</u>)	High
Experimental	NR	25 °C	13.4 atm-m ³ /mol		(<u>NLM, 2020</u>)	High
Experimental	NR	20 °C	3.4	Undimensioned Henry's law constant was 3.4 ±1.37 (grand mean over 5 experiments)	(<u>Hamelink et al.,</u> 1996)	High
Experimental; Not reported	98.1% radiochemical purity	21.7 °C	2.70±0.14	log Kaw = 2.70 ± 0.14 ; Air = 0.417 mg/L; Water = 8.34×10^{-4} mg/L	(Xu and Kropscott, 2012)	High
Experimental; Not reported	98.1% radiochemical purity	21.6 °C	2.68	log Kaw = 2.68 ; ± 0.12 ; Air = 0.741 ; mg/L Water = 1.53×10^{-3} mg/L	(Xu and Kropscott, 2012)	High
Experimental	>99.9% (w/w)	10−25 °C	1.23–7.66	Mean Hc (undimensional) at temperatures of 10, 15, 20, 25°C were 1.35, 2.38, 2.98, 4.78, respectively. Mean recoveries were 79.8, 80.9, 79.8, 84.5% for respective temperatures.	(Ann Arbor Technical Services, 2000 5889409)	High
Experimental	>99.9% (w/w)	20 °C	0.98–4.10	Mean Hc (undimensional) at 4, 8, 16, 32 μg/L starting concentration were 2.96, 3.53, 1.91, 2.98, respectively. Mean recoveries were 82.0, 80.5, 82.9, 79.8% for respective starting concentrations.	(Ann Arbor Technical Services, 2000 5889409)	High
Experimental	>99.9% (w/w)	20 °C	2.21–8.88	Mean Hc (undimensional) at 24, 48, 72, 96, 120 hours were 4.60, 5.62, 7.77, 5.04, 3.42, respectively. Mean recoveries were 91.6, 101.9, 88.2,	(Ann Arbor Technical Services, 2000 5889409)	High

Study Type	Substance Purity	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
				79.0, 78.6% for respective equilibration time.		
Experimental	>99.9% (w/w)	20 °C	13.83–19.41	mean of 3 values 17.0; mean recovery 89.9±3.7%	(Ann Arbor Technical Services, 1990 5889489)	High
Experimental	99.9%	28 °C (301 K)	≥23 to ≤24	Static head space method and modified batch air stripping method (vapor entry loop method VEL) used for direct measurement of Henry's law constant.	(<u>Kochetkov et al.,</u> 2001)	High

Table 11. Flash Point Study Summary for D4

Study Type	Substance Purity	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	131 °F	55 °C		(NLM, 2020)	High
Experimental	NR	NR	56 °C		(NLM, 2020)	High
Experimental	NR	NR	57 °C		(RSC, 2020)	High
Experimental	NR	NR	56 °C		(RSC, 2020)	High
Experimental	NR	NR	56 °C		(RSC, 2020)	High
Experimental	NR	NR	54 °C		(<u>RSC, 2020</u>)	High

Table 12. Auto Flammability Study Summary for D4

No Autoflammability data was identified for this chemical.

Table 13. Viscosity Study Summary for D4

Study Type	Apparatus	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental		25–25.1°C	2.187–2.239 cP	13 values were reported in Reaxys; 4 values were reported in the range of 2.187–2.239 cP at 25–25.1 °C; 9 values were outside this range or measured at unreported or non-standard temperatures.	(<u>Elsevier</u> , 2019)	High
Experimental		25 °C	2.30 сР	Reported as 2.30 cSt	(NLM, 2020)	High
Experimental		293.15 K	2.45 mPa.s	Reported as 2.45 mPa-s at 293.15 K; ranged from 2.45–0.41 mPa-s at 293.15–423.15 K.	(<u>Palczewska-</u> Tulinska and Oracz, 2005)	High
Experimental		300 K	2.7 mPa.s		(Liu et al., 2013)	High

Table 14. Refractive Index Study Summary for D4

Study Type	Apparatus	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	20 °C/D	1.3968		(<u>O'Neil,</u> 2013)	High
Experimental	19.99–25 °C	1.3935–1.4013	22 values were reported in Reaxys; 15 values were reported in the range of 1.3935–1.4013 at 19.99–25 °C; 7 values were outside this range or measured at unreported or non-standard temperatures.	(<u>Elsevier,</u> 2019)	High
Not specified	20 °C/D	1.3968		(<u>Haynes,</u> 2014)	High
Experimental	NR	1.396		(<u>RSC, 2020</u>)	High
Experimental	NR	1.396		(<u>RSC</u> , 2020)	High
Experimental	20 °C/D	1.3968		(<u>NLM,</u> 2020)	High
Experimental	293.15K	1.39674	Reported as 1.39674 at 293.15 K; also measured at 1.38925–1.37917 over 308.15-328.15 K, respectively.	(<u>Zhang et al., 2015</u>)	High

Table 15. Dielectric Constant Study Summary for D4

Study Type	Apparatus	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	20 °C	2.4–2.405	Static Dielectric Constant	(<u>Elsevier</u> , 2019)	High

EPI SuiteTM Model Outputs (U.S. EPA, 2012)

SMILES: C[Si]1(C)O[Si](C)(C)O[Si](C)(C)O[Si](C)(C)O1

CHEM: OCTAMETHYLTETRASILOXANE

MOL FOR: C8 H24 O4 Si4

MOL WT: 296.62

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

Physical Property Inputs: Log Kow (octanol-water): 6.49 Boiling Point (°C C): 175.80 Melting Point (°C): 17.50 Vapor Pressure (mm Hg): 1.05 Water Solubility (mg/L): 0.056 Henry LC (atm-m3/mole): 12

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1.68 estimate) = 6.79 Log Kow (Exper. database match) = 6.74 Exper. Ref: SEHSC (2009); average

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

Boiling Pt (°C): 159.41 (Adapted Stein & Brown method)

Melting Pt (°C): 1.78 (Mean or Weighted MP)

VP(mm Hg,25 °C): 1.18 (Mean VP of Antoine & Grain methods) VP (Pa, 25 °C): 158 (Mean VP of Antoine & Grain methods)

MP (exp database): 17.5 °C BP (exp database): 175.8 °C

VP (exp database): 1.05E+00 mm Hg (1.40E+002 Pa) at 25 °C

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

Water Solubility at 25 °C (mg/L): 0.1083

log Kow used: 6.49 (user entered)

melt pt used: 17.50 °C

Water Sol (Exper. database match) = $0.005 \text{ mg/L} (25 ^{\circ}\text{C})$

Exper. Ref: DOW CORNING (1987)

Water Sol Estimate from Fragments: Wat Sol (v1.01 est) = 0.17229 mg/L

ECOSAR Class Program (ECOSAR v1.11):

Class(es) found: Neutral Organics

Henry's Law Constant (25 °C) [HENRYWIN v3.20]:

Bond Method: 8.72E-002 atm-m3/mole (8.84E+003 Pa-m3/mole)

Group Method: Incomplete

Exper Database: 1.17E-01 atm-m3/mole (1.19E+004 Pa-m3/mole)

For Henry LC Comparison Purposes:

User-Entered Henry LC: 1.200E+001 atm-m3/mole (1.216E+006 Pa-m3/mole) Henry's LC [via VP/WSol estimate using User-Entered or Estimated values]:

HLC: 7.318E+000 atm-m3/mole (7.415E+005 Pa-m3/mole)

VP: 1.05 mm Hg (source: User-Entered) WS: 0.056 mg/L (source: User-Entered)

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

Log Kow used: 6.49 (user entered) Log Kaw used: 2.691 (user entered)

Log Koa (KOAWIN v1.10 estimate): 3.797 Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model): 0.6063 Biowin2 (Non-Linear Model): 0.2309 Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.5437 (weeks-months) Biowin4 (Primary Survey Model): 3.4198 (days-weeks)

MITI Biodegradation Probability: Biowin5 (MITI Linear Model): -0.1670 Biowin6 (MITI Non-Linear Model): 0.0028 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 Dec C)[AEROWIN v1.00]:

Vapor pressure (liquid/subcooled): 140 Pa (1.05 mm Hg)

Log Koa (Koawin est): 3.797

Kp (particle/gas partition coef. (m3/ug)):

Mackay model: 2.14E-008

Octanol/air (Koa) model: 1.54E-009

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model: 7.74E-007

Mackay model: 1.71E-006

Octanol/air (Koa) model: 1.23E-007

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

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 1.1968 E-12 cm3/molecule-sec

Half-Life = 8.937 Days (12-hr day; 1.5E6 OH/cm3)

Half-Life = 107.246 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

1.24E–006 (Junge-Pankow, Mackay avg)

1.23E-007 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc: 1.444E+004 L/kg (MCI method)

Log Koc: 4.159 (MCI method)

Koc: 4.271E+005 L/kg (Kow method)

Log Koc: 5.631 (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 = 3.948 (BCF = 8867 L/kg wet-wt)

Log Biotransformation Half-life (HL) = 1.6572 days (HL = 45.41 days)

Log BCF Arnot-Gobas method (upper trophic) = 3.982 (BCF = 9592)

Log BAF Arnot-Gobas method (upper trophic) = 6.122 (BAF = 1.324e+006)

log Kow used: 6.49 (user entered)

Volatilization from Water:

Henry LC: 12 atm-m3/mole (entered by user) Half-Life from Model River: 1.758 hours

Half-Life from Model Lake: 163.6 hours (6.816 days)

Removal in Wastewater Treatment (recommended maximum 95%):

Total removal: 99.91 percent

Total biodegradation: 0.18 percent Total sludge adsorption: 59.87 percent

Total to Air: 39.86 percent (using 10000 hr Bio P,A,S)

Level III Fugacity Model:

Mass Amount Half-Life Emissions

	(percent)	(hr)	(kg/hr)
Air	31	254	1000
Water	39.2	900	1000
Soil	1.42	1.8e + 003	1000
Sediment	28.5	8.1e+003	0

Persistence Time: 214 hr

Data Evaluation Tables

Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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 / 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	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	RSC (2020). ChemS ₁	pider: D4. HERO II	D:6982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Physical State reported by this reference. Cited reference: OU Chemical Safety Data.

Study Reference:	NLM (2020). PubChem	database: compo	und summary: D4. HERO ID:	6982832	}	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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 / 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
Test Reliability	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Physical State reported by this reference.

Cited reference: Lewis, R.J. Sr.; Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY 2007., p. 918

Study Reference:	NLM (2020). PubChem	database: compour	nd summary: D4. HERO ID:6	982832		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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)	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Physical State reported by this reference.

Cited reference: O'Neil, M.J. (ed.). The Merck Index – An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1255.

Study Reference:	RSC (2020). ChemSp	ider: D4. HERO I	D:6982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
		•	Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Physical Properties reported by this reference. Cited reference: OU Chemical Safety Data.

	Veighted Score
Substance Appropriateness High Measured data are consistent with the subject chemical substance in the subject chemical substance structural features or other physical/chemical properties or behaviors. Reliability / Unbiased (Method Objectivity) Medium There is no indication that the methodology for producing the information was biased towards a particular product or outcome. Reliability / Analytical Method Medium 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. Databases High The information or data is from a recognized data collection/	_
Substance Substance Substance Appropriateness High Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1
Consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1
Reliability / Unbiased (Method Objectivity)	
Method unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source. Databases High The information or data 1 1 is from a recognized data collection/	2
is from a recognized data collection/	2
Other are peer-reviewed by experts in the field, are broadly available to the public for review and use.	1
Models NR Rating of this factor is not applicable to this kind of information.	NR
Sum of scores: 7 5	7
High Medium Low Overall Score = Sum of Weighted Score (Rounded):	1.4
≥1 and <1.7 ≥1.7 and <2.3 ≥2.3 and ≤3 Overall Quality Level: The reviewer agreed with the overall rating for the Physical Properties reported by this reference.	High

Study Reference:	NLM (2020). PubChen	ı database: compo	und summary: D4. HERO	ID:6982	832	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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)	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	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	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	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7		≥2.3 and ≤3	Properties reported by this		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Physical Properties reported by this reference. Cited reference: ILO International Chemical Safety Cards (ICSC).

Study Reference:	NLM (2020). PubChen	n database: comp	ound summary: D4. HERO	ID:69828	332	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	Unacceptable	Measured data are not consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. It is not likely to be a powder with a melting point of 18 °C.	4	1	4
	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
Test Reliability	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	10	5	10
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	2	Overall Score (Rounded):	4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Unacceptable ¹

Physical state (dry powder) is inconsistent with subject chemical substance melting point of 18°C. Consistent with our Application of Systematic Review in TSCA Risk Evaluation document, if a metric for a data source receives a score of Unacceptable (score = 4), EPA will determine the study to be unacceptable. In this case, one of the metrics was rated as unacceptable. As such, the study is considered unacceptable and the score is presented solely to increase transparency. Cited reference: EPA Chemicals under the TSCA.

Study	Fuller, J; White, D; Yi, I					
Reference:	undesirable odors in a po			cycled pl	astic resin with	solid-phase
	microextraction. Chemo		EKU ID:0834323			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])		Metric Score	Metric Weighting Factor	Weighted Score
Cubatanaa	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	The odor intensity was determined qualitatively by pretrained people based on a 1–10 scale.	2	1	2
	Reliability / Analytical Method	Low	Odor assessment was not the focus of the primary study, and only qualitative determination was used.	3	1	3
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
ouiti	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	3	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	2	Overall Score (Rounded):	2
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall rati	≥2.3 and ≤3			Overall Quality Level:	Medium

Study Reference:	U.S. EPA (2020). Chem		formation for D4. HERO	ID:69828	26	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference. Cited reference: Data range determined from multiple primary sources in Chemistry Dashboard.

Reference:	index: An encyclopedia		s, and biologicals. HERO ID:	6982970		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or	1	1	1
			estimated for the subject chemical substance.			
	Appropriateness	High	Measured data are consistent	1	1	1
Substance	Appropriateness	Ingn	with the subject chemical	1	1	1
			substance structural features			
			or other physical/chemical			
			properties or behaviors.			
	Reliability / Unbiased	Medium	There is no indication that	2	1	2
	(Method Objectivity)		the methodology for			
			producing the information			
			was biased towards a			
			particular product or			
Test	D 1: 1:1:4 / A 1 4: 1	3.6.11	outcome.		1	2
Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be	2	1	2
	Method		appropriate based on the			
			data's inclusion in a peer-			
			reviewed/recognized			
			database or other secondary			
			source.			
	Databases	High	The information or data is	1	1	1
			from a recognized data			
			collection/repository where			
			data are peer-reviewed by			
Other			experts in the field, are			
			broadly available to the			
	Models	NR	public for review and use. Rating of this factor is not	NR	NR	NR
	Models	INIX	applicable to this kind of	INIX	INIX	INIX
			information.			
	ı		Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of	1.4	Overall	1.4
			Weighted Scores/Sum of		Score	
			Metric Weighting Factors:		(Rounded):	
≥ 1 and $\leq 1.\overline{7}$	\geq 1.7 and \leq 2.3	≥2.3 and ≤3		·	Overall	High
					Quality	
			Point reported by this reference		Level:	

Study	Elsevier (2019). Reaxys HERO ID:6984075	: physical-chemical	property data for D4. CAS R	Registry	Number: 556-	67-2.
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Cub stance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	5 Overall Score (Rounded):	7 1.4
	≥1.7 and <2.3	≥2.3 and ≤3	Point reported by this reference		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference. Cited reference: Data range determined from multiple primary sources in REAXYS.

Reference:	HERO ID:6982969					1
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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)	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	NLM (2020). PubChem	database: compour	nd summary: D4. HERO ID:6	982832		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
Total	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
Test Reliability	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Cited reference: EPA DSSTox; Hazardous Substances Data Bank (HSDB); ILO International Chemical Safety Cards (ICSC)

Study Reference:	RSC (2020). ChemSpid	er: D4. HERO ID:69	982833			
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's physical/chemical properties.	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	5 Overall Score (Rounded):	7 1.4
	≥1.7 and <2.3	≥2.3 and ≤3	Point reported by this reference		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference. Cited reference: Strem Product Catalog: https://www.strem.com/catalog/v/14-5400/.

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	V V		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference. Cited reference: Sigma-Aldrich.

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	9 9 24		Overall Quality Level:	High

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

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
T 4	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
T 4	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer- reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference. Cited reference: Jean-Claude Bradley Open Melting Point Dataset.

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
(Method Objectiv	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Uigh	Medium	Low	Sum of scores: Overall Score = Sum of	7 1.4	5 Overall Score	7 1.4
High	Medium	LOW	Weighted Scores/Sum of Metric Weighting Factors:	1.4	(Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Melting Point reported by this reference. Cited reference: OU Chemical Safety Data (no longer updated).

Study Reference:	Component Properties f	or a Few Siloxanes	ders, S., Gmehling, J. Mea Used as Working Fluids f earch. 2011. 50:9748. HER	or Orga	nic Rankine Cy	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) and/or other physical/chemical properties.	1	1	1
	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
Test Reliability	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/recognize d database or other secondary source.	2	1	2
	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer	agreed with the overall rat	ing for the Melting F	Point reported by this refere	nce.		

Study Reference:	U.S. EPA (2020). Chem	istry dashboard info	ormation for D4. HERO ID:6	982826		
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
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	7 1.4	5 Overall Score (Rounded):	7 1.4
	≥1.7 and <2.3	≥2.3 and ≤3	Point reported by this reference		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Boiling Point reported by this reference. Cited reference: Data range determined from multiple primary sources in Chemistry Dashboard.

Study Reference:	O'Neil, M. J. (2013). Th HERO ID:6982970	e Merck Index D4.	Cambridge, UK, The Royal S	ociety o	f Chemistry.	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	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.	1	1	1
N	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
High		Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	7 1.4	5 Overall Score (Rounded):	7 1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer	agreed with the overall ra	ating for the Boiling	Point reported by this reference			

Study Reference:	O'Neil, M. J. (2013). Th HERO ID:6982970	e Merck Index D4.	Cambridge, UK, The Royal S	ociety o	f Chemistry.	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	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.	1	1	1
N	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
High		Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	7 1.4	5 Overall Score (Rounded):	7 1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer	agreed with the overall ra	ating for the Boiling	Point reported by this reference			

Study Reference:	Elsevier (2019). Reaxys HERO ID:6984075	: physical-chemical	property data for D4. CAS	Registry	Number: 556-	67-2.
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
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	Test Reliability Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Boiling Point reported by this reference. Cited reference: Data range determined from multiple primary sources in REAXYS.

Domain	HERO ID:6982969	Qualitative				
	Metric	Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
]	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
	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.	1	1	1
Mod	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:		5 Overall Score (Rounded):	7 1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	NLM (2020). PubChen	n database: comp	ound summary: D4. HERO ID:69	82832		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
	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
Test Reliability	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	<u> </u>		Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Cited reference: O'Neil, M.J. (ed.). The Merck Index – An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1255.

Study Reference:	NLM (2020). PubChem	database: compour	nd summary: D4. HERO ID:6	982832		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
(Method Object	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Cited reference: O'Neil, M.J. (ed.). The Merck Index – An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1255.

Study Reference:									
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score			
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1			
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1			
TD4	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			
Test Reliability	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	1	1	1			
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR			
High	Medium	Low	Sum of scores: Overall Score = Sum of	7	5 Overall	7 1.4			
			Weighted Scores/Sum of Metric Weighting Factors:		Score (Rounded):				
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High			

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

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
(Method O	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Boiling Point reported by this reference. Cited reference: Strem Product Catalog: https://www.strem.com/catalog/v/14-5400/.

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	982833			
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
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	5 Overall Score (Rounded):	7 1.4
	≥1.7 and <2.3	≥2.3 and ≤3	Point reported by this reference		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Boiling Point reported by this reference. Cited reference: Sigma-Aldrich.

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	V V		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Boiling Point reported by this reference. Cited reference: LabNetwork.

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:	982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
(Method)	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	7 1.4	5 Overall Score (Rounded):	7 1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Boiling Point reported by this reference. Cited reference: Oakwood.

Study Reference:	RSC (2020). ChemSpic	der: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
Test Reliability Reliab	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference:	RSC (2020). ChemSpid	ler: D4. HERO ID:	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Boiling Point reported by this reference. Cited reference: OU Chemical Safety Data (no longer updated).

Study Reference:	O'Neil, M. J. (2013). Th HERO ID:6982970	ne Merck Index D4.	Cambridge, UK, The Royal S	Society o	of Chemistry.	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
6.1.4	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer	agreed with the overall ra	ating for the Density	reported by this reference.			

Study	Elsevier (2019). Reaxy HERO ID:6984075	ys: physical-chemi	cal property data for D4.	. CAS Re	gistry Number	r: 556-67-2.
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
Substance Appro	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
	≥1.7 and <2.3	≥2.3 and ≤3	sity reported by this refere		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Density reported by this reference. Cited reference: Data range determined from multiple primary sources in REAXYS.

Reference:	HERO ID:6982969	T	1		ı	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
6.1.4	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥ 1 and < 1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	NLM (2020). PubChem	database: compour	nd summary: D4. HERO ID:6	982832		
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
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
The sale	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
Test Reliability	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Cited reference: O'Neil, M.J. (ed.). The Merck Index – An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry, 2013., p. 1255.

Study Reference:	NLM (2020). PubCho	em database: compo	und summary: D4. HERO) ID:698	2832	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject	1	1	1
			chemical substance.			
Substance	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
/	la c 41	1-	Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:		Overall Score (Rounded):	1.5
	≥1.7 and <2.3	≥2.3 and ≤3	ty raported by this reference		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Density reported by this reference. Cited reference: ILO International Chemical Safety Cards (ICSC).

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
G I A	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Density reported by this reference. Cited reference: Sigma-Aldrich.

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:	982833			
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
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
4	la c	I.	Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:	982833			
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
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
4	la c	I.	Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
C-l-4	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	Ŭ Ü		Overall Quality Level:	High

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

Study Reference:		ane, D4, and decam	Selected physicochemica ethylcyclopentasiloxane. 0:3569075			d
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	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
Test Reliability	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
O.I	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	3	3	3
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer	agreed with the overall rati	ing for the Density re	eported by this reference.			

Study Reference:	tris(3,3,3-trifluoropropy	Zhang, Y; Dong, H; Wu, C; Yu, L; Xu, J. (2015). The mixing properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl) cyclotrisiloxane with various organosilicon compounds at different temperatures. The Journal of Chemical Thermodynamics 81: 16–25. HERO ID:4279677							
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			
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR			
	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			
Test Reliability	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			
	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR			
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR			
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	3			
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall ration	≥2.3 and ≤3			Overall Quality Level:	High			

Study Reference:	U.S. EPA (2020). Chem	istry dashboard info	ormation for D4. HERO ID:6	982826		
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
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
T. 4	Reliability / Unbiased (Method Objectivity)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a recognized, peer- reviewed data collection. Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	2 2		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Vapor Pressure reported by this reference. Cited reference: Physprop.

Study Reference:	NLM (2020). PubChem		nd summary: D4. HERO I	D:69828	32	
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)	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	ressure reported by this refer		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Vapor Pressure reported by this reference. Cited reference: EPA DSSTox; Hazardous Substances Data Bank (HSDB).

Study Reference:	NLM (2020). PubChem		ound summary: D4. HERO II	0:6982832		
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)	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
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	J		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Vapor Pressure reported by this reference. Cited reference: ILO International Chemical Safety Cards (ICSC).

Study Reference:	Lei, YD; Wania, F; Mathers, D, an. (2010). Temperature-Dependent Vapor Pressure of Selected Cyclic and Linear Polydimethylsiloxane Oligomers. Journal of Chemical and Engineering Data 55: 5868–5873. HERO ID:2629388						
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score	
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1	
Substance	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	
Othor	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	4 Overall Score (Rounded):	1	
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High	
The reviewer	agreed with the overall rat	ing for the Vapor Pre	ssure reported by this refer	rence.	•		

Study Reference:	Flaningam, O. L. (1986) and Engineering Data 3			e) oligome	rs. Journal of C	Chemical
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.	1	1	1
(Method Objectivity)	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	Low	Data are obtained by accepted standard analytical methods. Score reduced because all measurements were outside of environmental range.	3	1	3
	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	4	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.75	Overall Score (Rounded):	1.8
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Medium
The reviewer	agreed with the overall rat	ing for the Vapor Pro	essure reported by this re	ference.		

Study Reference:	U.S. EPA (2020). Chem	istry dashboard inf	ormation for D4. HERO ID:6	982826		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
(Method Object	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
Database 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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Water Solubility reported by this reference. Cited reference: Physprop; Kovdienko, et. al. Molecular informatics 29.5 (2010): 394–406.

Study		xys: physical-chemic	cal property data for D4. CA	S Registi	ry Number: 5	556-67-2.
Domain	HERO ID:6984075 Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	Unacceptable	Data measured for the subject chemical substance are not consistent with the subject chemical substance structural properties, features or behaviors.	4	1	4
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
			Sum of scores:	10	5	10
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	2	Overall Score (Rounded):	4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Unacceptable ^a

"The value was determined to be misreported in the secondary source when compared to the primary source. Consistent with our Application of Systematic Review in TSCA Risk Evaluation document, if a metric for a data source receives a score of Unacceptable (score = 4), EPA will determine the study to be unacceptable. In this case, one of the metrics was rated as unacceptable. As such, the study is considered unacceptable and the score is presented solely to increase transparency. Cited reference: Varaprath S et al; Environ Toxicol Chem 15(8): 1263–1265 (1996).

Study Reference:	NLM (2020). PubChem	ı database: compoi	and summary: D4. HERO	ID:6982	2832	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	Unacceptable	Source reports as none which may indicate the compound was not tested.	4	1	4
Substance	Appropriateness	Low	Data measured for the subject chemical substance are not consistent with the subject chemical substance structural properties, features or behaviors.	3	1	3
Test Reliability Reliab	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	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
041	Databases	High	Data is from a recognized, peer- reviewed data collection.	1	1	1
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	12	5	12
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	2.4	Overall Score (Rounded):	4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Unacceptable ^a

^a Consistent with our Application of Systematic Review in TSCA Risk Evaluation document, if a metric for a data source receives a score of Unacceptable (score = 4), EPA will determine the study to be unacceptable. In this case, one of the metrics was rated as unacceptable. As such, the study is considered unacceptable and the score is presented solely to increase transparency.

Cited reference: ILO International Chemical Safety Cards (ICSC).

Study Reference:	NLM (2020). PubChem	database: compour	nd summary: D4. HERO ID:	5982832		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
(Method Objectivity)	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Water Solubility reported by this reference. Cited reference: ECHA; Search for Chemicals. D4 (CAS 556-67-2) Registered Substances Dossier. European Chemical Agency. Available from, as of Aug 17, 2015: http://echa.europa.eu/.

Study Reference:	NLM (2020). PubChen	n database: compo	und summary: D4. HERO II	0:6982832	;	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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 Reliab	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Water Solubility reported by this reference. Cited reference: Varaprath S et al; Environ Toxicol Chem 15(8): 1263–1265 (1996)

Reference: Domain	Toxicology and Chemist Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or	Comments	Metric Score	Metric Weighting Factor	Weighted Score
		Not Rated [NR])				
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
Reliability / Unbiased (Method Objectivity) Test Reliability / Analytical Reliability Method	· ·	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.	1	1	1
	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	
0.4	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	2		Overall Quality Level:	High

Study Reference:	INDEPROOF BUILDING THE CLASS BUILDING TO THE CLASS OF THE CONTRACT OF THE CONT						
Domain	Metric 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)	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 described in limited detail but is expected to be appropriate.	2	1	2	
041	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
	I	_	Sum of scores:	6	4	6	
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5	
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall rate	≥2.3 and ≤3			Overall Quality Level:	High	

Study Reference:							
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score	
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1	
Substance	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)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2	
2-02-10-2	Reliability / Analytical Method	Medium	The analytical method is described in limited detail but is expected to be appropriate.	2	1	2	
	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
			Sum of scores:	6	4	6	
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5	
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	olubility reported by this re		Overall Quality Level:	High	

Study Reference:	Gee, RP. (2015). Emulsion polymerization of dimethylcyclosiloxane in cationic emulsion: Mechanism study utilizing two phase liquid-liquid reaction kinetics. Colloid Surface Physicochem Eng Aspect 481: 297–306. HERO ID:6833841						
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score	
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1	
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1	
Toot	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	
	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
			Sum of scores:	4	4	4	
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1	
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High	
The reviewer	agreed with the overall ra	ating for the Water So	blubility reported by this re	ference.			

747_306 HERO 11)•6	0330.44		iysicocii	em Eng Aspe	ct 481:
<u>297–306. HERO ID:6</u> Metric	Qualitative Determination (i.e., High, Medium, Low,	Comments	Metric Score	Metric Weighting Factor	Weighted Score
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
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
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
		Sum of scores:	4	4	4
Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
	Representativeness Appropriateness Reliability / Unbiased (Method Objectivity) Reliability / Analytical Method Databases Models Medium	Metric Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR]) Representativeness High Appropriateness High Reliability / Unbiased (Method Objectivity) High Reliability / Analytical Method High Databases NR Models NR Medium Low ≥1.7 and <2.3	Metric Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR]) Comments Representativeness High Data are measured or estimated for the subject chemical substance. Appropriateness High Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. 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. 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. Databases NR Rating of this factor is not applicable to this kind of information. Models NR Rating of this factor is not applicable to this kind of information. Medium Low Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	Metric Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR]) Data are measured or estimated for the subject chemical substance. Appropriateness High Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. 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. Reliability / Analytical Method Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or another developed standard. NR applicable to this kind of information. NR applicable to this kind of information. NR applicable to this kind of information. Sum of scores: 4 Medium Low Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	Metric Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR]) Comments Metric Score Metric Weighting Factor Representativeness High Data are measured or estimated for the subject chemical substance. 1 1 Appropriateness High Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. 1 1 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 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 Databases NR Rating of this factor is not applicable to this kind of information. NR NR Models NR Rating of this factor is not applicable to this kind of information. NR NR Medium Low Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors: 4 4 Medium Low Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors: Overall O

Study Reference:		es, D4 - determination	on of the water solubility in	syntheti	ic seawater. 19	989.
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
Test I	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
Othor	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	Springborn Laboratorio HERO ID:5889414	es, D4 - determination	on of the water solubility in	freshwa	ter. 1989.	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1
Substance	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
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	Bayer AG, Contribution HERO ID:5899898	s on assessment of th	ne aquatic toxicity of OM	ICTS wi	th cover letter.	1990.
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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)	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 non- standard but is expected to be appropriate.	2	1	2
Oth on	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer	agreed with the overall rati	ng for the Water Solu	bility reported by this refe	erence.		

Study Reference:	Bayer AG, Contribution HERO ID:5899898	ns on assessment of	the aquatic toxicity of (OMCTS wi	ith cover letter.	1990.
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)	Medium	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	2	1	2
rendomey	Reliability / Analytical Method	Medium	The analytical method is non- standard but is expected to be appropriate.	2	1	2
Othor	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall rat	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	Rhone-Poulenc Inc. Env HERO ID:5899916	vironmental fate of	D4 with cover letter. 19	990.		
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 / Unbiased (Method Objectivity)	Low	The methodology indicates that method bias is likely.	3	1	3
Reliability	Reliability / Analytical Method	Low	The analytical method described is not appropriate.	3	1	3
	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	8	4	8
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	2	Overall Score (Rounded):	2
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	, , , , , , , , , , , , , , , , , , , ,		Overall Quality Level:	Medium

Study Reference:	Rhone-Poulenc Inc, Env HERO ID:5899916	rironmental fate of D	4 with cover letter. 1990	0.		
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 / Unbiased (Method Objectivity)	Low	The methodology indicates that method bias is likely.	3	1	3
Reliability	Reliability / Analytical Method	Low	The analytical method described is not appropriate.	3	1	3
O/I	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	8	4	8
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	2	Overall Score (Rounded):	2
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall rat	≥2.3 and ≤3			Overall Quality Level:	Medium

Reference:	092987. 1987. HERO ID	Qualitative				
Domain	Metric	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 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).	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	High	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	Medium	Analytic method is non-standard but is expected to be appropriate.	2	1	2
041	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	5	4	5
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.25	Overall Score (Rounded):	1.3
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	Dow Corning, The water HERO ID:5905954	r solubility of D4 with	attachments and cove	r letter o	lated 092987. 19	987.
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups).	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	High	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 analytic methods.	1	1	1
O.I.	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	Springborn, L. (1989). (freshwater. Washington					y in
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
	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
Test Reliability	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
Othor	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	4 Overall Score (Rounded):	1
	≥1.7 and <2.3	\geq 2.3 and \leq 3	··· January I detoils.		Overall	High

Study Reference:	Dow Corning, Aqueous	solubility studies of	D4. 1991. HERO ID:731	0465		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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
041	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall	High

Study Reference:	, , , ,	emistry dashboard info	ormation for D4. HERO ID:698.	2826		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])		Metric Score	Metric Weighting Factor	Weighted Score
Cub atom as	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	2	1	2
O4I	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	2 2		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Octanol Water Coefficient (logKow) reported by this reference. Cited reference: Physprop.

Study	Elsevier (2019). Reaxys: HERO ID:6984075	physical-chemical	property data for D4. C.	AS Registry	y Number: 556-	67-2.
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Octanol Water Coefficient (logKow) reported by this reference. Cited reference: Data range determined from multiple primary sources in REAXYS.

Study Reference:	NLM (2020). PubChem	n database: compou	nd summary: D4. HERO ID:6	5982832		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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)	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
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:		Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Octanol Water Coefficient (logKow) reported by this reference. Cited reference: Xu S et al; Environ Sci Technol 48: 11748–11759 (2014).

Study Reference:	Xu, S. and B. Kropscott (2014). Evaluation of the three-phase equilibrium method for measuring temperature dependence of internally consistent partition coefficients (KOW, KOA, and KAW) for volatile methylsiloxanes and trimethylsilanol. Environmental Toxicology and Chemistry 33(12): 2702–2710. HERO ID:2535012							
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score		
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1		
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1		
	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		
Test Reliability	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		
Omer	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR		
			Sum of scores:	4	4	4		
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1		
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall rat	≥2.3 and ≤3			Overall Quality Level:	High		

Study Reference:	Xu, S. and B. Kropscott cyclic volatile methylsild 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
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
	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
Test Reliability	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
0.1	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall rat	≥2.3 and ≤3			Overall Quality Level:	High

Reference:	092987. 1987. HERO ID					
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups).	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	High	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 analytic methods.	1	1	1
Othon	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	9		Overall Quality Level:	High

Study Reference:	Dow Corning, Subject: M HERO ID:7310176	Monthly summary 1	0/1982, octanol-water o	coefficier	nts. 1982.	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	NR	Data are measured for the subject chemical substance.	NR	NR	NR
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.	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	High	Data are obtained by accepted standard analytical methods.	1	1	1
	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	3	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.3	Overall Score (Rounded):	1.3
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer	agreed with the overall ratio	ng for the Octanol W	ater Coefficient (logKov	v) reporte	ed by this referen	ce.

Study Reference:	Kozerski, G., Shawl, H. slow-stirring method usi				icient of D4 (D4) by the
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.	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.	1	1	1
O.I.	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall rati	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	U.S. EPA (2020). Chem	istry dashboard inf	ormation for D4. HERO	ID:698282	6	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
Test	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	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Henry's Law reported by this reference. Cited reference: Physprop.

Study Reference:	Xu, S. and B. Kropscott (2014). Evaluation of the three-phase equilibrium method for measuring temperature dependence of internally consistent partition coefficients (KOW, KOA, and KAW) for volatile methylsiloxanes and trimethylsilanol. Environmental Toxicology and Chemistry 33(12): 2702–2710. HERO ID: 2535012						
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).	1	1	1	
Test Reliability	Reliability / Unbiased (Method Objectivity)	High	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	Analytic method is non-standard but is expected to be appropriate.	2	1	2	
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
	I	I	Sum of scores:	5	4	5	
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.25	Overall Score (Rounded):	1.3	
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High	
	≥1.7 and <2.3 agreed with the overall rat			erence.	Quality	Hi	

Reference:		Qualitative				
Domain	Metric	Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
	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
Test Reliability	Reliability / Analytical Method	Medium	The analytical method is unknown but is the analytical method is unknown but is likely to be appropriate likely to be appropriate based on the data's inclusion in a peerreviewed/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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
·			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Henry's Law reported by this reference. Cited reference: Xu S, Kropscott B; Environ Toxicol Chem 33(12): 2702–10 (2014).

Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not rated)	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
	≥1.7 and <2.3 r agreed with the overall ra	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Henry's Law reported by this reference. Cited reference: EPA DSSTox.

Study			(1996). Henry's law cons			and
Reference: Domain	aquatic half-life of D4. E Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
	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
Test Reliability	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
041	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	g g		Overall Quality Level:	High

Study Reference:			imultaneous determination ilanediol. Analytical Chem			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance's 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	Medium	The analytical method is non- standard but is expected to be appropriate.	2	1	2
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Otner	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	5	4	5
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.25	Overall Score (Rounded):	1.3
	≥1.7 and <2.3	≥2.3 and ≤3	aw reported by this reference		Overall Quality Level:	High

Medium, Low, Unacceptable, or Not Rated [NR] Data are measured or estimated for the subject chemical substance. I	Study Reference:	HERO ID:2188633							
Substance Appropriateness High Measured data are consistent with the subject chemical substance's other physical/chemical properties or behaviors. Reliability / Unbiased (Method Objectivity) Reliability / Analytical Method Reliability / Analytical Method Method Method Medium The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear. Reliability / Analytical Method Method Method NR Rating of this factor is not applicable to this kind of information. Models NR Rating of this factor is not applicable to this kind of information. Sum of scores: Medium Low Overall Scores Sum of Metric Weighting Factors: Overall Quality Overall Quality Overall Quality	Domain	Metric	Determination (i.e., High, Medium, Low, Unacceptable, or	Comments		Weighting	Weighted Score		
Consistent with the subject chemical substance's other physical/chemical properties or behaviors.		Representativeness	High	estimated for the subject	1	1	1		
Contex	Substance	Appropriateness	High	consistent with the subject chemical substance's other physical/chemical	1	1	1		
Reliability / Analytical Method Medium The analytical method is non- standard but is expected to be appropriate. 2 1 2 Databases NR Rating of this factor is not applicable to this kind of information. NR NR			High	producing the information is designed to answer a specific question, and the methodology's objective	1	1	1		
DatabasesNRRating of this factor is not applicable to this kind of information.NRNRNRModelsNRRating of this factor is not applicable to this kind of information.NRNRNRSum of scores:545HighMediumLowOverall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:1.25Overall Score (Rounded): ≥ 1 and $\langle 1.7 \rangle \geq 1.7$ and $\langle 2.3 \rangle \geq 2.3$ and ≤ 3 ≥ 2.3 and ≤ 3 Overall Overall Overall Ouality	•		Medium	The analytical method is non- standard but is expected to be	2	1	2		
Models NR Rating of this factor is not applicable to this kind of information. NR NR NR NR NR NR NR N	O.I.	Databases	NR	Rating of this factor is not applicable to this kind of	NR	NR	NR		
High Medium Low Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	Otner	Models	NR	Rating of this factor is not applicable to this kind of information.		NR	NR		
		_	_						
\geq 1 and \leq 1.7 and \leq 2.3 and \leq 3 Overall Quality High	High	Medium	Low	Weighted Scores/Sum of Metric Weighting	1.25	Score	1.3		
The reviewer agreed with the overall rating for the Henry's Law reported by this reference.							High		

Study Reference:	Ann Arbor Technical So HERO ID:5889409	ervices, Inc., Phase I	I studies of the Henry's	law cons	tant of OMCTS	(D4). 2000
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	1	1	1
	Reliability / Analytical Method	High	The analytical method is non-standard but is expected to be appropriate.	1	1	1
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
TT' 1	N. 11		Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall rat	≥2.3 and ≤3			Overall Quality Level:	High

Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	1	1	1
	Reliability / Analytical Method	High	The analytical method is non- standard but is expected to be appropriate.	1	1	1
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	Ann Arbor Technical S HERO ID:5889409	ervices, Inc., Phase I	I studies of the Henry's	law consta	ant of OMCTS ((D4). 2000.
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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	There is no indication that the methodology for producing the information was biased towards a particular product or outcome.	1	1	1
Kenability	Reliability / Analytical Method	High	The analytical method is non- standard but is expected to be appropriate.	1	1	1
	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	4	4	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
	≥1.7 and <2.3 agreed with the overall ra	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	Ann Arbor Technical S HERO ID:5889489		's law constant of OMC	.15 (D4) a	ι 20 degrees. 19	790.
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
	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
Fest Reliability	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
041	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	4 Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	Kochetkov, A., et al. (20) Toxicology and Chemist			ic metny	i siloadiles. Liivi	ii omnemu
Domain	Metric Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])		Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured for the subject chemical substance.	1	1	1
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features.	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 non-standard but is expected to be appropriate.	2	1	2
Othon	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	I	1-	Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall rati	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	NLM (2020). PubChem	n database: compo	ound summary: D4. HERO I	D:698283	2	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Carla at a sa a a	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	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
Test Reliability	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.	1	1	1
Mo	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Flash Point reported by this reference. Cited reference: ILO International Chemical Safety Cards (ICSC).

Study Reference:	NLM (2020). PubChem	database: compour	nd summary: D4. HERO ID:6	982832		
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
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
The sale	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
Test Reliability	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:		Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Flash Point reported by this reference. Cited reference: Sigma-Aldrich; Safety Data Sheet for D4. Product Number: 235695, Version 3.14 (Revision Date 02/28/2015). Available from, as of September 30, 2015: http://www.sigmaaldrich.com/safety-center.html.

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Cubatanaa	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Test	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Flash Point reported by this reference. Cited reference: LabNetwork.

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not rated)	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Carlo et a ma a	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer- reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Flash Point reported by this reference. Cited reference: Oakwood.

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Curk atomor	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/ recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference:	RSC (2020). ChemSpid	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Cubatanaa	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Flash Point reported by this reference. Cited reference: OU Chemical Safety Data (no longer updated).

keierence:	HERO ID:6984075	Qualitativa				
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
G 1 4	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance A	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Test Reliability Relia	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	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	NLM (2020). PubChem	database: compour	nd summary: D4. HERO ID:6	982832		
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
Substance	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Viscosity reported by this reference. Cited reference: Hazardous Substances Data Bank (HSDB).

Study Reference:	Palczewska-Tulinska, M hexamethylcyclotrisilox Engineering Data 50: 1'	ane, D4, and decar	nethylcyclopentasiloxaı			d
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)	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
O.I	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	3	3	3
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	9 9		Overall Quality Level:	High

Study Reference:			of confined liquids using	the thern	nal bending fluc	tuations of
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
C-1-4	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	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
Test Reliability	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
	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	3	3	3
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1	Overall Score (Rounded):	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

Study Reference:	O'Neil, M. J. (2013). TI HERO ID:6982970	he Merck Index D	4. Cambridge, UK, The Roya	l Society o	of Chemistry.	
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
6.1.4	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Togs	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer	agreed with the overall r	ating for the Refrac	ctive Index reported by this refe	erence.		

Study Reference:	Elsevier (2019). Reaxys HERO ID:6984075	s: physical-chemic	al property data for D4	. CAS Reg	istry Number	: 556-67-2.
Domain	Metric 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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Refractive Index reported by this reference. Cited reference: Data range determined from multiple primary sources in REAXYS.

	HERO ID:6982969	Qualitative Determination		Matri	Metric	11 700-1-4
Domain	Metric	(i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Weighting Factor	Weighted Score
	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	V g		Overall Quality Level:	High

Study Reference:	RSC (2020). ChemSpid	er: D4. HERO ID:69	982833			
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
Subsunce	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	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
Test Reliability	Reliability / Analytical Method	Medium	Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer- reviewed/recognized database or other secondary source.	2	1	2
Other	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	I	-	Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Refractive Index reported by this reference. Cited reference: Sigma-Aldrich.

Study Reference:	RSC (2020). ChemSpid	er: D4. HERO ID:6	982833			
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
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Test	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	, , , , , , , , , , , , , , , , , , , ,		Overall Quality Level:	High

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

Study Reference:	NLM (2020). PubChem	database: compour	nd summary: D4. HERO ID:6	5982832		
Domain	Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Substance	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.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	7		Overall Quality Level:	High

The reviewer agreed with the overall rating for the Refractive Index reported by this reference. Cited reference: Hazardous Substances Data Bank (HSDB).

Study Reference:	tris(3,3,3-trifluoropropy	Zhang, Y; Dong, H; Wu, C; Yu, L; Xu, J. (2015). The mixing properties of 1,3,5-trimethyl-1,3,5-tris(3,3,3-trifluoropropyl) cyclotrisiloxane with various organosilicon compounds at different temperatures. The Journal of Chemical Thermodynamics 81: 16–25. HERO ID:4279677							
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			
	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			
Test Reliability	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			
	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR			
Other	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR			
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	3	Overall Score (Rounded):	3			
≥1 and <1.7	≥1.7 and <2.3 agreed with the overall ratio	≥2.3 and ≤3		f.	Overall Quality Level:	High			

Study	Elsevier (2019). Reaxys HERO ID:6984075	s: physical-chemic	al property data for D4. CA	S Registry	y Number: 556-	67-2.
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 Relia	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	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	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Dielectric Constant reported by this reference. Cited reference: Data range determined from multiple primary sources in REAXYS.

Study			erface Suite TM for Microsoft®	Window	ws, v 4.11 (Co	mputer
Reference: Domain	Program). Washingt Metric	Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
G 1 4	Representativeness	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
Substance	Appropriateness	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
Test	Reliability / Unbiased (Method Objectivity)	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
Reliability	Reliability / Analytical Method	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
	Databases	NR	The metric is not applicable to this study type (SAR).	NR	1	NR
Other	Models	High	The models in EPI Suite TM have defined endpoints. Chemical domain and performance statistics for each model are known, and unambiguous algorithms are available in the EPI Suite TM documentation and/or cited references to establish their scientific validity. Many EPI Suite TM models have correlation coefficients >0.7, cross-validated correlation coefficients >0.5, and standard error values <0.3; however, correlation coefficients (r², q²) 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
High	Medium	Low	Sum of scores: Overall Score = Sum of	1 1	Overall	1
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3	Weighted Scores/Sum of Metric Weighting Factors:		Score (Rounded): Overall Quality Level:	High

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