

Draft 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



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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		(<u>NLM, 2020</u>)	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		(<u>NLM, 2020</u>)	Unacceptable
Experimental	Colorless, oily liquid		(<u>NLM, 2020</u>)	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
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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		(<u>O"Neil, 2013</u>)	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.	(<u>Elsevier, 2019</u>)	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, 2020</u>)	High
Experimental	NR	17.5–18 °C		(<u>RSC, 2020</u>)	High
Experimental	NR	17–18 °C		(<u>RSC, 2020</u>)	High
Experimental	NR	17–18 °C		(<u>RSC, 2020</u>)	High
Experimental	NR	17–18 °C		(<u>RSC, 2020</u>)	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.	(<u>Abbas et al., 2011</u>)	High

	Table 4.	Boiling	Point Study	Summary	for	D4
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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	(<u>O'Neil, 2013</u>)	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		(<u>NLM, 2020</u>)	High
Experimental	NR	74 °C	20 mm Hg	(<u>NLM, 2020</u>)	High
Experimental	NR	175 °C		(<u>NLM, 2020</u>)	High
Experimental	NR	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
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	(<u>O'Neil, 2013</u>)	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/cm ³ at 19.99-25 °C; 26 values were outside this range or measured at unreported or non-standard temperatures.	(<u>Elsevier, 2019</u>)	High
Experimental			20 °C	0.9561		(<u>Haynes, 2014</u>)	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, 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, 2020</u>)	High
Experimental			292.00 K	0.95755	Reported as 957.55 kg/m ³ at 292.00 K; 957.55– 790.24 kg/m ³ at 292.00–433.15 K	(<u>Palczewska-</u> <u>Tulinska and</u> <u>Oracz, 2005</u>)	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	(<u>Zhang et al.,</u> <u>2015</u>)	High

Table 6. Vapor Pressure Study Summary for D ⁴	Table 6.	Vapor	Pressure	Study	Summary	for	D4
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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> <u>2020</u>)	High
Experimental	NR	25 °C	1.05 torr	Reported as 1.05 mm Hg	(<u>NLM,</u> <u>2020</u>)	High
Experimental	NR	21.7 °C	133.3 Pa		(<u>NLM,</u> <u>2020</u>)	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> <u>2010</u>)	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> <u>1986</u>)	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	рН	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>U.S. EPA,</u> <u>2020</u>)	High
Experimental	NR	23 °C	NR			Reported as 189.86E6 mmol/L	(<u>Elsevier, 2019</u>)	Unacceptable
Experimental	NR	23°C	NR		0.056 mg/L		(<u>NLM, 2020</u>)	High
Experimental	NR	25 °C	NR		0.033 mg/L	Measured in synthetic seawater	(<u>NLM, 2020</u>)	High
Experimental	NR	NR	NR			Reported as "none"	(<u>NLM, 2020</u>)	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</u> <u>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> <u>1995</u>)	High
Experimental; Column generator	>99%	NR	NR		0.033 mg/L	Reported as 33 µg/L in saltwater	(<u>Sousa et al.,</u> <u>1995</u>)	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.	(<u>Springborn</u> <u>Laboratories,</u> <u>1989c</u>)	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	(<u>Springborn</u> <u>Laboratories</u> , <u>1989b</u>)	High

Study Type	Substance Purity	Temperature	рН	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	(<u>Bayer AG,</u> <u>1990</u>)	High
Experimental	NR	25 °C	NR		27–33 µg/L	Mean value 29.5 µg/L	(<u>Bayer AG,</u> <u>1990</u>)	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.	(<u>Rhone-Poulenc</u> <u>Inc, 1990</u>)	Medium
Experimental	NR	20 °C	NR		15–240 ppb	It is impossible to deduce a precise value from the present results.	(<u>Rhone-Poulenc</u> Inc, 1990)	Medium
Experimental	>99.5%	NR	NR		50 ррb	Water solubility determined as a result of log Kow measurement. First determination: 25 ppb in water; second determination: 53 ppb in water	(<u>Dow Corning,</u> <u>1987a</u>)	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.	(<u>Dow Corning,</u> <u>1987b</u>)	High
Experimental; Non-Turbulent Partitioning of D4	>99% Pure	23 °C	NR		56 ppb	WS ranged from 50–60 ppb	(<u>Dow Corning,</u> <u>1991</u>)	High

Study Type	Substance Purity	Temperature	рН	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	(<u>Springborn</u> <u>Laboratories</u> , <u>1989a</u>)	High

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

Study Type	Substance Purity	Temperature	рН	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> <u>2020</u>)	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> <u>2019</u>)	High
Experimental	NR	NR	NR	NR	6.74	Average of three measurements	(<u>NLM,</u> <u>2020</u>)	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	(<u>Xu and</u> <u>Kropscott,</u> <u>2014</u>)	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	(<u>Xu and</u> <u>Kropscott,</u> <u>2012</u>)	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	(<u>Kozerski</u> <u>and Shawl,</u> <u>2007</u>)	High
Experimental	>99%	NR	NR	OECD classical partitioning between 50 mL octanol and 250 mL water	4.0		(<u>Dow</u> <u>Corning,</u> <u>1982</u>)	High
Experimental	>99.5%	NR	NR	$100 \ \mu L \ (0.0956 \ g) D4 \ in 25 \ g \ (30.23 \ mL) octanol placed in a 250 \ mL Wheaton bottle with 150 \ mL distilled water. The bottle was capped, agitated for an hour on a Burrell wrist-action shaker, and allowed to settle overnight.$	5.10		(<u>Dow</u> <u>Corning,</u> <u>1987a</u>)	High

Table 10. Henry's Law Cons	tant Study Summary f	or D4
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Study Type	Substance Purity	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	NR	12.0 atm-m ³ /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> <u>1996</u>)	High
Experimental; Not reported	98.1% radiochemical purity	21.7 °C	2.70±0.14	log Kaw = 2.70 \pm 0.14; Air = 0.417 mg/L; Water = 8.34 \times 10 ⁻⁴ mg/L	(<u>Xu and</u> <u>Kropscott, 2012</u>)	High
Experimental; Not reported	98.1% radiochemical purity	21.6 °C	2.68	log Kaw = 2.68; \pm 0.12; Air = 0.741; mg/L Water = 1.53×10^{-3} mg/L	(<u>Xu and</u> <u>Kropscott, 2012</u>)	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.	(<u>Ann Arbor</u> <u>Technical</u> <u>Services, 2000</u> <u>5889409</u>)	High
Experimental	>99.9% (w/w)	20 °C	0.98–4.10	Mean Hc (undimensional) at 4, 8, 16, 32 μ g/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.	(<u>Ann Arbor</u> <u>Technical</u> <u>Services, 2000</u> <u>5889409</u>)	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,	(<u>Ann Arbor</u> <u>Technical</u> <u>Services, 2000</u> <u>5889409</u>)	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%	(<u>Ann Arbor</u> <u>Technical</u> <u>Services, 1990</u> <u>5889489</u>)	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> <u>2001</u>)	High

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

Table 11. Flash Point Study Summary for D4

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, 2019</u>)	High
Experimental		25 °C	2.30 cP	Reported as 2.30 cSt	(<u>NLM, 2020</u>)	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> <u>Tulinska and Oracz,</u> <u>2005</u>)	High
Experimental		300 K	2.7 mPa.s		(<u>Liu et al., 2013</u>)	High

Table 14	. Refractive	Index Study	^v Summary	for D4
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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> <u>2019</u>)	High
Not specified	20 °C/D	1.3968		(<u>Haynes,</u> <u>2014</u>)	High
Experimental	NR	1.396		(<u>RSC, 2020</u>)	High
Experimental	NR	1.396		(<u>RSC, 2020</u>)	High
Experimental	20 °C/D	1.3968		(<u>NLM,</u> <u>2020</u>)	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</u> <u>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, 2019</u>)	High

EPI SuiteTM Model Outputs

(<u>U.S. EPA, 2012</u>)

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) = 6.79Log Kow (Exper. database match) = 6.74Exper. 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 mg/L (25 °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 Amou	int Half-Life E	missions	
	(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

Study	O'Neil, M. J. (2013). Th	ne Merck Index D4.	Cambridge, UK, The Royal S	Society o	f Chemistry.	
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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
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	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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer	agreed with the overall r	ating for the Physica	l State reported by this referenc	e		

Study Reference:	RSC (2020). ChemS	pider: D4. HERO II	D:6982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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
Study Reference: Domain Substance Fest Reliability Other High >1 and <1.7	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
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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited referen	agreed with the overall ce: OU Chemical Safet	rating for the Physic y Data.	cal State reported by this rel	ference.		

Study Reference:	NLM (2020). PubChem	database: compo	und summary: D4. HERO ID:	6982832	2	
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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
			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 Cited referenc New York, N	agreed with the overall ra e: Lewis, R.J. Sr.; Hawle Y 2007., p. 918.	ting for the Physica y's Condensed Che	l State reported by this reference mical Dictionary 15th Edition. J	e. Iohn Wil	ey & Sons, Inc	2.

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>i.e.</i> , 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
			chemical substance.			
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
Tort	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	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
TT' 1		¥	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 ra	ating for the Physical	State reported by this reference	e.		

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>i.e.</i> , 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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited referen	agreed with the overall ce: OU Chemical Safety	rating for the Physi Data.	ical Properties reported by the	is reference	е.	

Study Reference:	O'Neil, M. J. (2013). TI HERO ID:6982970	he Merck Index I	04. Cambridge, UK, The	e Royal	Society of Ch	emistry.
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	1	1	1
Substance			consistent with the			
			subject chemical			
			features or other			
			physical/chemical			
			properties or behaviors.			
	Reliability / Unbiased	Medium	There is no indication	2	1	2
	(Method Objectivity)		that the methodology			
			for producing the			
			information was biased			
			towards a particular			
			product or outcome.			
Test Reliability	Reliability / Analytical	Medium	Analytical method is	2	1	2
	Method		unknown but is likely to			
			be appropriate based on			
			the data's inclusion in a			
			recognized database or			
			other secondary source			
	Databases	High	The information or data	1	1	1
	Databases	mgn	is from a recognized	1	1	1
			data collection/			
			repository where data			
			are peer-reviewed by			
Other			experts in the field, are			
Other			broadly available to the			
			public for review and			
			use.			
	Models	NR	Rating of this factor is	NR	NR	NR
			hot applicable to this			
			Sum of scores	7	5	7
High	Medium	Low	Overall Score – Sum	1 /	Overall	1 /
111811	i i cululli	200	of Weighted	1.+	Score	1.7
			Scores/Sum of Metric		(Rounded):	
			Weighting Factors:		· · · · · · · · · · · · · · · · · · ·	
≥ 1 and < 1.7	≥1.7 and <2.3	≥ 2.3 and ≤ 3			Overall	High
					Quality	-
					Level:	
The reviewer agreed w	ith the overall rating for the	he Physical Proper	rties reported by this refer	ence.		

Study	NLM (2020). PubChen	n database: compo	und summary: D4. HERC) ID:6982	832	
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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
Test Rehability	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	≥1.7 and <2.3	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer ag Cited reference:	reed with the overall rati ILO International Chem	ng for the Physical I ical Safety Cards (I	Properties reported by this CSC).	reference.		

Study	NLM (2020). PubChen	ı database: comp	ound summary: D4. HERO	ID:69828	332	
Reference:						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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
Tost	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	\geq 2.3 and \leq 3			Overall Quality Level:	Unacceptable ¹
Physical state Application of Unacceptable unacceptable Cited referen	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 Jnacceptable (score = 4), EPA will determine the study to be unacceptable. In this case, one of the metrics was rated as inacceptable. 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	H; Colley, J; Vickery, Z	Z; Liu, S. (2020). Ana	lysis of v	olatile compoun	ds causing
Reference:	undesirable odors in a p	White, D; Yi, H; Colley, J; Vickery, Z; Liu, S. (2020). Analysis of volatile compounds cale odors in a polypropylene - high-density polyethylene recycled plastic resin with solid-critics. Chemosphere 260: 127589. HERO ID:6834323 Ietric Qualitative Determination (i.e., High, Medium, Low, Unacceptable, or Not Rated [NR]) Comments Metric Score Metric Weighting Factor Weighting Factor ativeness High Data are measured or estimated for the subject chemical substance. 1 1 1 teness NR Rating of this factor is not applicable to this kind of information. NR NR NR / Unbiased Medium The odor intensity 2 1 1 / Analytical Low Odor assessment was anot the focus of the primary study, and only qualitative determination was used. 3 1 / Analytical Low Odor assessment was anot the focus of the primary study, and only qualitative determination was used. NR NR NR NR Rating of this factor is not applicable to this kind of information. NR NR NR / Analytical Low Odor assessment was anot the focus of the primary study, and only qualitative determination was used. 1 1 / Analytical NR Rating of this factor is not applicable to this kind of informati	solid-phase			
	microextraction. Chemo	sphere 260: 127589. H	ERO ID:6834323	-	1	
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Test	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
Test	Reliability / Unbiased (Method Objectivity)	Medium	The odor intensity was determined qualitatively by pretrained people based on a 1–10 scale.	2	1	2
Reliability	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
Other	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	$\geq 2.3 \text{ and } \leq 3$		G	Overall Quality Level:	Medium
The reviewer	agreed with the overall rati	ng for the Physical Prot	perties reported by this	reference	2	

Study Reference:	U.S. EPA (2020). Chemistry dashboard information for D4. HERO ID:6982826							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
i ne reviewei	agreed with the overall ra	ating for the Melting	point reported by this ref	erence.				

Cited reference: Data range determined from multiple primary sources in Chemistry Dashboard.

Study	O'Neil, M. J. (2013). The Merck Index D4. Cambridge, UK, The Royal Society of Chemistry. The Merck						
Reference:	index: An encyclopedia	for chemicals, drug	s, and biologicals. HERO ID:	6982970			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score	
Substance	Representativeness	High	Data are measured or estimated for the subject	1	1	1	
	Appropriateness	High	chemical substance. Measured data are consistent with the subject chemical substance structural features or other physical/chemical	1	1	1	
	Reliability / Unbiased (Method Objectivity)	Medium	properties or behaviors. There is no indication that the methodology for producing the information was biased towards a particular product or	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:	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.

Study Reference:	y Elsevier (2019). Reaxys: physical-chemical property data for D4. CAS Registry Number: 556-67-2. https://doi.org/10.1016/084075						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score	
C-b-t	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 race: Data range determined	ating for the Melting	Point reported by this reference ary sources in REAXYS	e.			

Study Reference:	Study Haynes, W. M. (2014). CRC Handbook of Chemistry and Physics D4. Boca Raton, FL, CRC Press.								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score			
Substance	Representativeness	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	\geq 1.7 and <2.3	≥ 2.3 and ≤ 3			Overall Quality Level:	High			
The reviewer	agreed with the overall ra	ting for the Melting P	oint reported by this reference	e.		•			

Study	NLM (2020). PubChem	database: compour	nd summary: D4. HERO ID:6	982832			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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				
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical	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 Melting Point reported by this reference. Cited reference: EPA DSSTox; Hazardous Substances Data Bank (HSDB); ILO International Chemical Safety Cards (ICSC)							

Study Defenses	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			
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 Cited referen	agreed with the overall race: Strem Product Catalog	ating for the Melting I g: https://www.strem.	Point reported by this reference com/catalog/v/14-5400/.	2.					
Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833						
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Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score			
Substance	Representativeness	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			
			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	\geq 2.3 and \leq 3			Overall Quality Level:	High			
The reviewer Cited reference	The reviewer agreed with the overall rating for the Melting Point reported by this reference.								

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	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
			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	\geq 2.3 and \leq 3	~ ~		Overall Quality Level:	High
The reviewer Cited reference	agreed with the overall rat ce: LabNetwork.	ing for the Melting	Point reported by this refe	erence.		

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:	5982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	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
			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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited reference	agreed with the overall rate	ing for the Melting	Point reported by this refer	rence.		

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	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
			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 Cited reference	agreed with the overall rat	ing for the Melting	Point reported by this refer	rence.		

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	982833						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score			
Substance	Representativeness	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			
			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	\geq 2.3 and \leq 3			Overall Quality Level:	High			
The reviewer Cited reference	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:6	982833					
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score		
Substance	Representativeness	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		
			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 Cited reference	The reviewer agreed with the overall rating for the Melting Point reported by this reference.							

Study	Dbas, K., Schedemann, A., Ihmels, C., Enders, S., Gmehling, J. Measurement of Thermophysical Pure. Component Properties for a Few Siloxanes Used as Working Fluids for Organic Ranking Cycles							
Reference:	Industrial and Engineer	ing Chemistry Res	earch. 2011. 50:9748. HER	OF OF gal	110 Kankine Cy 335590	cies.		
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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 (<i>e.g.</i> , presence of certain functional groups) and/or other 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	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		
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR		
Utner	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	\geq 2.3 and \leq 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
		-	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 Cited referen	agreed with the overall race: Data range determined	ating for the Boiling I d from multiple prima	Point reported by this reference ary sources in Chemistry Dash	ooard.		

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>i.e.</i> , 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	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 ra	ating for the Boiling	Point reported by this reference			

Study O'Neil, M. J. (2013). The Merck Index D4. Cambridge, UK, The Royal Society of Chemistry. Reference: HFRO ID:6982970								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	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 ra	ating for the Boiling	Point reported by this reference					

Study Elsevier (2019). Reaxys: physical-chemical property data for D4. CAS Registry Number: 556-67-2.								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
Substance			estimated for the subject chemical 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.								

Study Poforonco:	Study Haynes, W. M. (2014). CRC Handbook of Chemistry and Physics D4. Boca Raton, FL, CRC Press.								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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 ra	ating for the Boiling l	Point reported by this reference						

Study	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832							
Reference:		0.114.11		1				
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
			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 Cited referen UK: Roval S	r agreed with the overall ince: O'Neil, M.J. (ed.). The ociety of Chemistry, 201	rating for the Boil he Merck Index – 3., p. 1255.	ing Point reported by this reference. An Encyclopedia of Chemicals, Dru	igs, and	Biologicals. C	ambridge,		

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>i.e.</i> , 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			
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors	1	1	1
TT (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 Cited referen	agreed with the overall race: O'Neil, M.J. (ed.). Th	ating for the Boiling I e Merck Index – An I	Point reported by this reference Encyclopedia of Chemicals, Dr	ugs, and	Biologicals. C	ambridge,

UK: Royal Society of Chemistry, 2013., p. 1255.

Study	Study NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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					
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1		
T4	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	\geq 2.3 and \leq 3			Overall Quality Level:	High		
The reviewer Cited referen	agreed with the overall race: EPA DSSTox.	ating for the Boiling	Point reported by this reference	2.				

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited reference	agreed with the overall rates e: Strem Product Catalog	ting for the Boiling l https://www.strem.	Point reported by this refer com/catalog/v/14-5400/.	rence.		

Study References	RSC (2020). ChemSpid	er: D4. HERO ID:6	982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited referen	agreed with the overall race: Sigma-Aldrich.	ating for the Boiling	Point reported by this reference			-

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited reference	agreed with the overall rat ce: LabNetwork.	ing for the Boiling I	Point reported by this refe	rence.		

Study Reference:	RSC (2020). ChemSpider: D4. HERO ID:6982833						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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 Cited reference	agreed with the overall rat	ing for the Boiling I	Point reported by this refere	ence.			

Study Reference:	RSC (2020). ChemSpic	ler: 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
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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited reference	agreed with the overall rate: Alfa Aesar.	ating for the Boiling I	Point reported by this refer	ence.		

Study Reference:	RSC (2020). ChemSpid	ler: D4. HERO ID:(5982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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			
Substance	Appropriateness	High	Measured data are consistent with the subject chemical's	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	Medium	physical/enemical physical/enemical physical/enemical 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 Cited referen	agreed with the overall race: OU Chemical Safety I	ating for the Boiling Data (no longer upda	Point reported by this refer ted).	ence.		

Study O'Neil, M. J. (2013). The Merck Index D4. Cambridge, UK, The Royal Society of Chemistry.								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score		
Sub store of	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	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		
TT' 1		Ŧ	Sum of scores:	6	4	6		
Hıgh	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	\geq 2.3 and \leq 3			Overall Quality Level:	High		
The reviewer	agreed with the overall r	ating for the Density	reported by this reference					

Study References	Study Elsevier (2019). Reaxys: physical-chemical property data for D4. CAS Registry Number: 556-67-2.								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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			
Tost	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:	<u>6</u> 1.5	4 Overall Score (Rounded):	<u>6</u> 1.5			
≥ 1 and < 1.7	\geq 1.7 and <2.3	\geq 2.3 and \leq 3			Overall Quality Level:	High			
The reviewer Cited referen	agreed with the overall ce: Data range determine	rating for the Dens red from multiple p	sity reported by this reference rimary sources in REAXY	nce. S.					

Study Reference:	Study Haynes, W. M. (2014). CRC Handbook of Chemistry and Physics D4. Boca Raton, FL, CRC Press. Reference: HERO ID:6082969								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score			
Substance	Representativeness	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	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 Weighted Scores/Sum of Metric Weighting Factors:	6 1.5	4 Overall Score (Rounded):	6 1.5			
≥ 1 and < 1.7	\geq 1.7 and \leq 2.3	≥ 2.3 and ≤ 3	reported by thisf		Overall Quality Level:	High			

Study Defense	ndy NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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			
Tort	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	\geq 2.3 and \leq 3			Overall Quality Level:	High			
The reviewer	agreed with the overall ra	ating for the Density	reported by this reference.		Dialagiasla (and and an			

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	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score			
Substance	Representativeness	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			
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting	6 1.5	4 Overall Score (Rounded):	6 1.5			
≥1 and <1.7	≥1.7 and <2.3	\geq 2.3 and \leq 3	Factors:		Overall Quality Level:	High			
The reviewer Cited referen	r agreed with the overal ace: ILO International C	ll rating for the Densit Chemical Safety Cards	ty reported by this reference s (ICSC).						

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited reference	agreed with the overall rat ce: Sigma-Aldrich.	ting for the Density	reported by this reference.			

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited reference	agreed with the overall rat ce: Fluorochem.	ing for the Density 1	reported by this reference.			

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	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 Cited reference	agreed with the overall rat	ing for the Density	reported by this reference.			

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	5982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited reference	agreed with the overall rat	ing for the Density	reported by this reference.			

Study Reference:	y hexamethylcyclotrisiloxane, D4, and decamethylcyclopentasiloxane. Journal of Chemical and Engineering Data 50: 1711–1719. HERO ID:3569075							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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)	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:	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	ng for the Density re	eported by this reference.					

Study	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							
Reference:								
	temperatures. The Jour	nal of Chemical Th	ermodynamics 81: 16–25	. HERO	ID:4279677			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score		
Substance	Representativeness	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		
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:	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	$\geq 2.3 \text{ and } \leq 3$			Overall Quality Level:	High		
The reviewer	agreed with the overall rati	ng for the Density re	eported by this reference.					

Study Reference:	U.S. EPA (2020). Chemistry dashboard information for D4. HERO ID:6982826							
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		
Substance	A	TT' - 1	chemical substance.	1	1	1		
	Appropriateness	High	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 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	\geq 2.3 and \leq 3			Overall Quality Level:	High		
The reviewer Cited referen	agreed with the overall race: Physprop.	ating for the Vapor Pr	essure reported by this reference	ce.				

Study Reference:	NLM (2020). PubChem	database: compour	nd summary: D4. HERO I	D:69828	32	
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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 Cited reference	agreed with the overall rat e: EPA DSSTox; Hazardo	ing for the Vapor Pr ous Substances Data	essure reported by this refer Bank (HSDB).	ence.		

Study	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832							
Reference:			11		1			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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.					
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 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			Overall Quality Level:	Hıgh		
The reviewer Cited referen	The reviewer agreed with the overall rating for the Vapor Pressure reported by this reference. Cited reference: ILO International Chemical Safety Cards (ICSC).							

Study	Lei, YD; Wania, F; Mathers, D, an. (2010). Temperature-Dependent Vapor Pressure of Selected Cyclic							
Reference	and Linear Polydimethylsiloxane Oligomers. Journal of Chemical and Engineering Data 55: 5868–5873.							
Kelerence.	HERO ID:2629388	1						
		Qualitative						
		Determination			Metric			
Domain	Metric	(<i>i.e.</i> , High,	Comments	Metric	Weighting	Weighted		
Domain	with	Medium, Low,	Comments	Score	Factor	Score		
		Unacceptable, or			1 actor			
		Not Rated [NR])						
	Representativeness	High	Data are measured for	1	1	1		
			the subject chemical					
			substance.					
	Appropriateness	High	Measured data are	1	1	1		
Substance			consistent with the					
Substance			subject chemical					
			substance structural					
			features or other					
			physical/chemical					
			properties or behaviors.					
	Reliability / Unbiased	High	The methodology for	1	1	1		
	(Method Objectivity)		producing the					
			information is designed					
			to answer a specific					
			question, and the					
			methodology's objective					
			is clear.					
Test	Reliability / Analytical	High	Data are obtained by	1	1	1		
Reliability	Method		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	NR	NR	NR		
			not applicable to this					
Other			kind of information.					
	Models	NR	Rating of this factor is	NR	NR	NR		
			not applicable to this					
			kind of information.					
xx* 1		Ŧ	Sum of scores:	4	4	4		
High	Medium	Low	Overall Score = Sum of	1	Overall Score	1		
			Weighted Scores/Sum		(Rounded):			
			of Metric Weighting					
. 1 1 1 - 1			Factors:			TT' 1		
≥ 1 and < 1.7	≥ 1.7 and < 2.3	≥ 2.3 and ≤ 3			Overall	Hıgh		
The					Quality Level:			
i ne reviewer	agreed with the overall rat	ing for the Vapor Pre	ssure reported by this refer	rence.				
Study	Flaningam, O. L. (1986). Vapor pressures of poly(dimethylsiloxane) oligomers. Journal of Chemical							
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Reference:	and Engineering Data 3	1(3): 266–272. HEI	KO ID:6989156					
Domain	Metric	Determination (<i>i.e.</i> , 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)	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		
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	M. 1'	T	Sum of scores:	175	4	7		
High	Medium	Low	of Weighted Scores/Sum of Metric Weighting Factors:	1.75	Overall Score (Rounded):	1.8		
≥ 1 and <1.7	≥1.7 and <2.3	\geq 2.3 and \leq 3			Overall Quality Level:	Medium		
The reviewer	agreed with the overall rat	ing for the Vapor Pro	essure reported by this re	terence.				

Study Reference:	ly U.S. EPA (2020). Chemistry dashboard information for D4. HERO ID:6982826							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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.					
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	\geq 2.3 and \leq 3			Overall Quality Level:	High		
The reviewer Cited referen	agreed with the overall race: Physprop; Kovdienko	ating for the Water So , et. al. Molecular inf	olubility reported by this reference or an arrest or a second state of the second stat	nce.				

Study Elsevier (2019). Reaxys: physical-chemical property data for D4. CAS Registry Number: 556-67-2. Reference: HERO ID:6984075								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	10 2	5 Overall Score (Rounded):	10 4		
≥ 1 and < 1.7	≥1.7 and <2.3	\geq 2.3 and \leq 3			Overall Quality Level:	Unacceptable ^a		
^{<i>a</i>} The value w our Applicati	as determined to be mis on of Systematic Revie	sreported in the seco w in TSCA Risk Ev	ndary source when compared aluation document, if a metric	to the print for a data	mary source. (a source received	Consistent with ves 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 database: compound summary: D4. HERO ID:6982832							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
The set	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		
	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		
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	<u>12</u> 2.4	5 Overall Score (Rounded):	4		
≥1 and <1.7	≥1.7 and <2.3	\geq 2.3 and \leq 3			Overall Quality Level:	Unacceptable ^{<i>a</i>}		
^a Consistent y receives a sc metrics was y transparency	with our Application of S ore of Unacceptable (scor rated as unacceptable. As 7.	ystematic Review ir ce = 4), EPA will der such, the study is co	1 TSCA Risk Evaluation doc termine the study to be unac onsidered unacceptable and	cument, i ceptable the score	f a metric for a . In this case, o e is presented s	a data source one of the olely to increase		

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

Study	NLM (2020). PubChem	database: compour	nd summary: D4. HERO ID:6	5982832		
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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.			
Substance	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1
T4	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 Cited referen	agreed with the overall race: ECHA; Search for Ch	ating for the Water Semicals. D4 (CAS 55	olubility reported by this refere 56-67-2) Registered Substances	nce. Dossier	. European Ch	emical

Agency. Available from, as of Aug 17, 2015: http://echa.europa.eu/.

Study	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832							
Reference:		[I			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
T (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 Cited referen	agreed with the overall r ce: Varaprath S et al; Env	ating for the Water viron Toxicol Chem	Solubility reported by this refe 15(8): 1263–1265 (1996)	erence.				

Study	Varaprath, S., et al. (1996). Aqueous solubility of permethylsiloxanes (silicones). Environmental							
Reference:	Toxicology and Chemist	try 15(8): 1263–126	5. HERO ID:6984031		1			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
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	\geq 2.3 and \leq 3			Overall Quality Level:	High		
The reviewer	agreed with the overall rati	ing for the Water So	lubility reported by this i	reference.				

Study	Sousa, JV; Mcnamara, PC; Putt, AE; Machado, MW; Surprenant, DC; Hamelink, JL; Kent, DJ;						
Reference:	Silberhorn, EM; Hobso	n, JF. (1995). Effec	ts of D4 (OMCTS) on fre	eshwater and	d marine orga	nisms.	
	Environ Toxicol Chem	14: 1639–1647. HE	RO ID:6834101		T		
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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.				
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	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	
Uner	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	\geq 2.3 and \leq 3			Overall Quality Level:	High	
The reviewer	agreed with the overall rat	ting for the Water So	plubility reported by this re	eference.			

Study	Study Sousa, JV; Mcnamara, PC; Putt, AE; Machado, MW; Surprenant, DC; Hamelink, JL; Kent, DJ;						
Reference	Silberhorn, EM; Hobson	n, JF. (1995). Effect	ts of D4 (OMCTS) on fres	shwater an	d marine orga	nisms.	
Kererence:	Environ Toxicol Chem	14: 1639–647. HER	O ID:6834101		T		
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	
		8	estimated for the subject chemical substance.				
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	The analytical method is described in limited detail but is expected to be appropriate.	2	1	2	
Others	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
Utner	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	\geq 2.3 and \leq 3			Overall Quality Level:	High	
The reviewer	agreed with the overall rat	ing for the Water Sc	olubility reported by this ref	ference.			

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:							
Domain	297–306. HERO ID:68 Metric	33841 Qualitative Determination (<i>i.e.</i> , 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		
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		
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	41	4 Overall Score (Rounded):	4 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	olubility reported by this ref	ference.				

Study	Gee, RP. (2015). Emu	Ilsion polymerization o	of dimethylcyclosiloxane in cation ion kinetics. Colloid Surface Pl	onic emu	Ilsion: Mecha	nism of 481.
Reference:	297–306. HERO ID:6	6833841	ion kineucs. Conoiu Surface Pi	rysicocii	em Eng Aspe	ci 401:
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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)	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
Ouler	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	\geq 1.7 and $<$ 2.3	\geq 2.3 and \leq 3	alubility reported by this reference		Overall Quality Level:	High

Study Reference:	Springborn Laboratories, D4 - determination of the water solubility in synthetic seawater. 1989.							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
Others	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:	4	4 Overall	4		
riigii		LOW	Weighted Scores/Sum of Metric Weighting Factors:	1	Score (Rounded):	1		
≥1 and <1.7	≥1.7 and <2.3	\geq 2.3 and \leq 3			Overall Quality Level:	High		

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

Study Reference:	Springborn Laboratories, D4 - determination of the water solubility in freshwater. 1989.							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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, Contributions on assessment of the aquatic toxicity of OMCTS with 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 / 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		
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:	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	ing for the Water Solu	bility reported by this ref	erence.				

Study Reference:	Bayer AG, Contributions on assessment of the aquatic toxicity of OMCTS with cover letter. 1990.								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	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			
	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		<u>c</u>	Overall Quality Level:	High			

Study Reference:	Rhone-Poulenc Inc. Environmental fate of D4 with cover letter. 1990. HERO ID:5899916								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score			
Substance	Representativeness	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			
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:	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	\geq 1.7 and $<$ 2.3	≥ 2.3 and ≤ 3	bubility apported by this	nofonon oc	Overall Quality Level:	Medium			

Reference:	HERO ID:5899916					
					1	
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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)	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
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:	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	bility reported by this	aron co	Overall Quality Level:	Medium

Study Reference:	Dow Corning. The n-oct 092987. 1987. HERO ID	anol/water partition c :5905948	coefficient of D4 with a	ttachme	nt and cover let	ter dated
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	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 (<i>e.g.</i> , 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
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
*** 1			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	\geq 1.7 and <2.3	≥ 2.3 and ≤ 3	ility appointed by this ast		Overall Quality Level:	High

Study Reference:	Dow Corning, The water solubility of D4 with attachments and cover letter dated 092987. 1987. : HERO ID:5905954							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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 (<i>e.g.</i> , 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		
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	\geq 1.7 and <2.3	\geq 2.3 and \leq 3	ility reported by this set	Coronao	Overall Quality Level:	High		

Study Reference:	Springborn, L. (1989). Octamethycyclotetrasiloxane – Determination of the water solubility in freshwater, Washington, DC, Silicones Health Council, HERO ID:7006395								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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			
	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:	4	4 Overall Score (Rounded):	4 1			
≥ 1 and < 1.7	≥1.7 and <2.3	≥ 2.3 and ≤ 3		- Com	Overall Quality Level:	High			

Study Reference:	Dow Corning, Aqueous solubility studies of D4. 1991. HERO ID:7310465							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score		
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1		
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors.	1	1	1		
Test Reliability	Reliability / Unbiased (Method Objectivity)	High	The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear.	1	1	1		
	Reliability / Analytical Method	High	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical- chemical properties or another developed standard.	1	1	1		
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR		
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR		
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	4	4 Overall Score (Rounded):	41		
≥ 1 and < 1.7	\geq 1.7 and <2.3	≥ 2.3 and ≤ 3			Overall Quality Level:	High		

Study	udy U.S. EPA (2020). Chemistry dashboard information for D4. HERO ID:6982826									
Reference:			Γ	1						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score				
Substance	Representativeness	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				
Others	Databases	High	Data is from a secondary database with a reference to the peer-reviewed original source.	1	1	1				
Otner	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	\geq 2.3 and \leq 3			Overall Quality Level:	High				
The reviewe	er agreed with the overa	all rating for the Octano	l Water Coefficient (logKow) repo	orted by	this reference.					

Study Reference:	Elsevier (2019). Reaxys: physical-chemical property data for D4. CAS Registry Number: 556-67-2. HERO ID:6984075							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	\geq 2.3 and \leq 3			Overall Quality Level:	High		
The reviewer Cited reference	agreed with the overall rat ce: Data range determined	ing for the Octanol V from multiple prima	Water Coefficient (logKow ry sources in REAXYS.) reported 1	by this reference			

Study Reference:	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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:	1.4	Overall Score (Rounded):	1.4		
≥ 1 and < 1.7	≥1.7 and <2.3	\geq 2.3 and \leq 3			Overall Quality Level:	High		
The reviewer Cited referen	agreed with the overall r ace: Xu S et al; Environ So	ating for the Octanol ci Technol 48: 11748	Water Coefficient (logKow) re 3–11759 (2014).	ported b	y this reference	e.		

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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>i.e.</i> , 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		
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR		
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	<u>4</u> 1	4 Overall Score (Rounded):	4 1		
≥ 1 and < 1.7	\geq 1.7 and $<$ 2.3	≥ 2.3 and ≤ 3	Water Coefficient (locV)	w) reported	Overall Quality Level:	High		

Study Reference:	Xu, S. and B. Kropscott (2012). Method for simultaneous determination of partition coefficients for cyclic volatile methylsiloxanes and dimethylsilanediol. Analytical Chemistry 84(4): 1948–1955. HERO ID:2188633							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
	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 rat	ing for the Octanol	Water Coefficient (logKo	ow) reported	by this reference	æ.		

Study Reference:	Dow Corning, The n-oct 092987. 1987. HERO ID	tanol/water partitio 9:5905948	on coefficient of D4 with	attachmei	nt and cover let	ter dated
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	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 (<i>e.g.</i> , 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
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	Water Coefficient (logKo) reported	Overall Quality Level:	High

Study Reference:	Dow Corning, Subject: Monthly summary 10/1982, octanol-water coefficients. 1982. e: HERO ID:7310176							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score		
Substance	Representativeness	NR	Data are measured for the subject chemical substance.	NR	NR	NR		
	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	\geq 1.7 and <2.3	\geq 2.3 and \leq 3			Overall Quality Level:	High		
The reviewer	agreed with the overall ration	ng for the Octanol Wa	ater Coefficient (logKov	v) reporte	d by this referen	ce.		

Study	Kozerski, G., Shawl, H. Determination of the 1-octanol/water partition coefficient of D4 (D4) by the						
Reference:	slow-stirring method usi	ng gas chromatograp	hy. 2007. HERO ID:6	987895			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	
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	$\geq 2.3 \text{ and } \leq 3$		`	Overall Quality Level:	High	
i ne reviewer	agreed with the overall rati	ng for the Octanol Wat	er Coefficient (logKow) reported	a by this reference	e.	

Study Reference:	U.S. EPA (2020). Chemistry dashboard information for D4. HERO ID:6982826						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score	
Substance	Representativeness	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	
			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	\geq 2.3 and \leq 3			Overall Quality Level:	High	
The reviewer Cited reference	agreed with the overall rat ce: Physprop.	ing for the Henry's l	Law reported by this refere	ence.			

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>i.e.</i> , 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 (<i>e.g.</i> , 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	
	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	
The reviewer	agreed with the overall rat	ing for the Henry's	Law reported by this refe	erence.			

Study	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832							
Reference:			Г Г		T			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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 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	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832							
Reference:		r						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
Tost	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	\geq 2.3 and \leq 3			Overall Quality Level:	High		
The reviewer Cited referen	agreed with the overall race: EPA DSSTox.	ating for the Henry's	Law reported by this refe	rence.				

Study	Hamelink, JL; Simon, PB; Silberhorn, EM. (1996). Henry's law constant, volatilization rate, and						
Reference:	aquatic half-life of D4. E	Environ Sci Technol	30: 1946–1952. HERO I	D:280312	24		
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	
Othon	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	
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	\geq 2.3 and \leq 3			Overall Quality Level:	High	
The reviewer	agreed with the overall rati	ing for the Henry's L	aw reported by this referen	nce.			

Study Reference: Xu, S. and B. Kropscott (2012). Method for simultaneous determination of partition coefficients for cyclic volatile methylsiloxanes and dimethylsilanediol. Analytical Chemistry 84(4): 1948–1955. HERO ID:2188633							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	
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	\geq 2.3 and \leq 3			Overall Quality Level:	High	

Study Reference:	Xu, S. and B. Kropscott (2012). Method for simultaneous determination of partition coefficients for cyclic volatile methylsiloxanes and dimethylsilanediol. Analytical Chemistry 84(4): 1948–1955. HERO ID:2188633							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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's other physical/chemical properties or behaviors.	1	1	1		
Test	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		
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		
The reviewer	agreed with the overall ration	ing for the Henry's I	Law reported by this referen	ce.				
Study Reference:	Ann Arbor Technical Services, Inc., Phase II studies of the Henry's law constant of OMCTS (D4). 2000. HERO ID:5889409							
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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)	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		
Othor	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		
High	Medium	Low	Sum of scores: Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	4	4 Overall Score (Rounded):	41		
≥ 1 and < 1.7	\geq 1.7 and $<$ 2.3	≥ 2.3 and ≤ 3	w reported by this refere	nce	Overall Quality Level:	High		

Study Reference:	Ann Arbor Technical Services, Inc., Phase II studies of the Henry's law constant of OMCTS (D4). 2000. :: HERO ID:5889409						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	
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 Quality Level:	High	

Study Reference:	Ann Arbor Technical Services, Inc., Phase II studies of the Henry's law constant 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 / 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	
	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	ting for the Henry's L	aw reported by this reference	ence.			

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

Study Reference:	Ann Arbor Technical Services, Inc., Henry's law constant of OMCTS (D4) at 20 degrees. 1990.							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	$\geq 2.3 \text{ and } \leq 3$			Overall Quality Level:	High		

Study	ly Kochetkov, A., et al. (2001). Air-water partition constants for volatile methyl siloxanes. Environmental						
Reference:	Toxicology and Chemist	ry 20(10): 2184–2188.	HERO ID:7303416	-			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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)	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	
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:	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	\geq 2.3 and \leq 3			Overall Quality Level:	High	
The reviewer	agreed with the overall ration	ng for the Henry's Law	reported by this refere	ence.			

Study Reference:	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
Cult store of			estimated for the subject 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		
			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 Cited referen	agreed with the overall r ce: ILO International Che	ating for the Flash emical Safety Card	Point reported by this references (ICSC).	ce.				

Study Reference:	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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.					
Substance	Appropriateness	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR		
Tost	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		
	1	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	≥ 2.3 and ≤ 3			Overall Quality Level:	High		

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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
Substance	Appropriateness	NR	chemical substance. 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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited reference	agreed with the overall rat	ing for the Flash Poi	nt reported by this referen	ce.		

Study Reference:	RSC (2020). ChemSpider: D4. HERO ID:6982833						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	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	\geq 2.3 and \leq 3			Overall Quality Level:	High	
The reviewer Cited reference	agreed with the overall rat ce: Oakwood.	ing for the Flash Poi	nt reported by this referen	ce.			

Study Reference:	RSC (2020). ChemSpide	er: D4. HERO ID:6	982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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
a 1 (estimated for the subject 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	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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited reference	agreed with the overall rat e: Alfa Aesar.	ing for the Flash Poi	nt reported by this referen	ce.		

Study Reference:	: RSC (2020). ChemSpider: D4. HERO ID:6982833						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	
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	\geq 2.3 and \leq 3			Overall Quality Level:	High	
The reviewer Cited reference	agreed with the overall rat e: OU Chemical Safety D	ing for the Flash Poi ata (no longer update	nt reported by this referenced).	ce.			

Study Reference:	Elsevier (2019). Reaxys HERO ID:6984075	: physical-chemic	al property data for D4.	CAS Registry]	Number: 556-	67-2.
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
Subsuite	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	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	\geq 1.7 and <2.3	≥ 2.3 and ≤ 3	sity reported by this refere	nce	Overall Quality Level:	High

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

Study Reference:	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832							
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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.					
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 Cited referen	agreed with the overall race: Hazardous Substances	ating for the Viscosit Data Bank (HSDB).	y reported by this reference.					

Study Reference:	Palczewska-Tulinska, M; Oracz, P. (2005). Selected physicochemical properties of hexamethylcyclotrisiloxane, D4, and decamethylcyclopentasiloxane. Journal of Chemical and Engineering Data 50: 1711–1719. HERO ID:3569075						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score	
Substance	Representativeness	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	
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR	
ottier	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	\geq 1.7 and $<$ 2.3	≥ 2.3 and ≤ 3	u reported by this referen	n co	Overall Quality Level:	High	

Study	Liu F et al. 2013. Atomic force microscopy of confined liquids using the thermal bending fluctuations of							
Reference:	the cantilever. Phys Rev	v E 87: 62406. HER	O ID:6835221					
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR		
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR		
		1	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 ra	ting for the Viscosity	v reported by this reference					

Study	Study O'Neil, M. J. (2013). The Merck Index D4. Cambridge, UK, The Royal Society of Chemistry.									
Reference:	HERO ID:6982970									
		Qualitative								
		Determination		Matuia	Metric	Weighted				
Domain	Metric	(<i>l.e.</i> , Hign, Madium I aw	Comments	Nietric	Weighting	veignied				
		Unaccontable or		Score	Factor	Score				
		Not Rated [NR])								
	Donrocontotivonoss	High	Data ara massurad or	1	1	1				
	Kepresentativeness	Ingn	astimated for the subject	1	1	1				
			chemical substance							
Substance	Annronriateness	NR	Rating of this factor is not	NR	NR	NR				
	Appropriateness		applicable to this kind of	INK						
			information							
	Reliability / Unbiased	Medium	There is no indication that the	2	1	2				
	(Method Objectivity)	1110010111	methodology for producing	-	-	_				
	(;)		the information was biased							
			towards a particular product							
T4			or outcome.							
l est Reliability	Reliability / Analytical	Medium	Analytical method is	2	1	2				
	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 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							
	Modola	ND	Pating of this factor is not	ND	ND	ND				
	wioueis	INK	applicable to this kind of	INK	INK	INK				
			information							
			Sum of scores:	б	4	6				
High	Medium	Low	Overall Score = Sum of	1.5	Overall	1.5				
		2011	Weighted Scores/Sum of	110	Score	110				
			Metric Weighting Factors:		(Rounded):					
≥ 1 and < 1.7	≥ 1.7 and < 2.3	≥ 2.3 and ≤ 3			Overall	High				
					Quality	Ŭ				
					Level:					
The reviewer	agreed with the overall r	ating for the Refrac	ctive Index reported by this refe	erence.		-				

Study Elsevier (2019). Reaxys: physical-chemical property data for D4. CAS Registry Number: 556-67-2.								
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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		
Substance			estimated for the subject chemical 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	\geq 2.3 and \leq 3			Overall Quality Level:	High		
The reviewer Cited referen	agreed with the overall r ce: Data range determine	ating for the Refra d from multiple pri	ctive Index reported by th imary sources in REAXY	is referenc S.	e			

Study	Study Haynes, W. M. (2014). CRC Handbook of Chemistry and Physics D4. Boca Raton, FL, CRC Press.								
Reference:	HERO ID:0982969	Orralitating	[
		Determination							
		(i.e. High		Matric	Metric	Weighted			
Domain	Metric	Modium Low	Comments	Score	Weighting	Score			
		Unaccontable or		Score	Factor	Score			
		Not Rated [NR])							
	Representativeness	High	Data are measured or	1	1	1			
	Representativeness	Ingn	estimated for the subject	1	1	1			
			chemical substance						
Substance	Annronriateness	NR	Rating of this factor is not	NR	NR	NR			
	rppioprateness		applicable to this kind of	THE	INK				
			information.						
	Reliability / Unbiased	Medium	There is no indication that the	2	1	2			
	(Method Objectivity)		methodology for producing						
			the information was biased						
			towards a particular product						
Test			or outcome.						
l est Reliability	Reliability / Analytical	Medium	The analytical method is	2	1	2			
	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 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						
		ND	public for review and use.	ND		ND			
	Models	NK	Rating of this factor is not	NK	NK	NK			
			applicable to this kind of						
			information.	6	4	6			
High	Madium	Low	Sum of scores:	0	4 Ovoroll	0			
Ingn	Wiedium	LOW	Weighted Scores/Sum of	1.3	Score	1.3			
			Metric Weighting Factors		(Rounded).				
>1 and <1 7	>1 7 and <2 3	>2.3 and <3	Free to the second seco		Overall	Hioh			
≥ 1 and ≤ 1.7					Onality	111611			
					Level:				
The reviewer	agreed with the overall ra	ating for the Refractiv	ve Index reported by this refere	nce.					

Study Reference:	RSC (2020). ChemSpid	er: D4. HERO ID:69	982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	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)	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	\geq 2.3 and \leq 3			Overall Quality Level:	High
The reviewer Cited referen	agreed with the overall race: Sigma-Aldrich.	ating for the Refractiv	e Index reported by this refere	nce.		

Study Reference:	RSC (2020). ChemSpid	er: D4. HERO ID:6	982833			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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	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 Cited referen	agreed with the overall race: Alfa Aesar.	ating for the Refractiv	ve Index reported by this refer	ence.		

Study Reference:	NLM (2020). PubChem database: compound summary: D4. HERO ID:6982832						
Domain	Metric	Qualitative Determination (<i>i.e.</i> , 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			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 Zhang, Y; Dong, H; Wu, C; Yu, L; Xu, J. (2015). The mixing properties of 1,3,5-trimethyl-1,3,5-						
Reference:	tris(3,3,3-trifluoropropy	l) cyclotrisiloxane wit	th various organosilico	n compou	unds at differen	t
Reference:	temperatures. The Journ	nal of Chemical Ther	modynamics 81: 16–25	. HERO	ID:4279677	
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	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
Other	Databases	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
	Models	NR	Rating of this factor is not applicable to this kind of information.	NR	NR	NR
			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	1 , 11 .1.		Overall Quality Level:	High
The reviewer	agreed with the overall rati	ng for the Refractive I	ndex reported by this ref	erence.		

Study	Elsevier (2019). Reaxys: physical-chemical property data for D4. CAS Registry Number: 556-67-2.							
Reference:	HERO ID:6984075				1			
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated [NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score		
Substance	Representativeness	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	$\geq 1.7 \text{ and } < 2.3$	≥ 2.3 and ≤ 3			Overall Quality Level:	High		
The reviewer Cited referen	agreed with the overall r ce: Data range determine	ating for the Diele d from multiple pri	ctric Constant reported by this imary sources in REAXYS.	reference.				

Study	U.S. EPA. (2012). Estimation Programs Interface Suite TM for Microsoft® Windows, v 4.11 (Computer							
Reference:	Program). Washingt	on, DC. HERO ID:2	2347246					
Domain	Metric	Qualitative Determination (<i>i.e.</i> , High, Medium, Low, Unacceptable, or Not Rated NR])	Comments	Metric Score	Metric Weighting Factor	Weighted Score		
	Representativeness	NR	The metric is not applicable	NR	1	NR		
Substance	Appropriateness	NR	to this study type (SAR). 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		
Kenadinty	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 (r^2 , q^2) for the regressions of some environmental fate models (<i>i.e.</i> , BIOWIN) are lower, as expected, compared to regressions which have specific experimental values such as water solubility or log Kow (octanol-water partition coefficient).	1	1	1		
			Sum of scores:	1	1	1		
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		

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