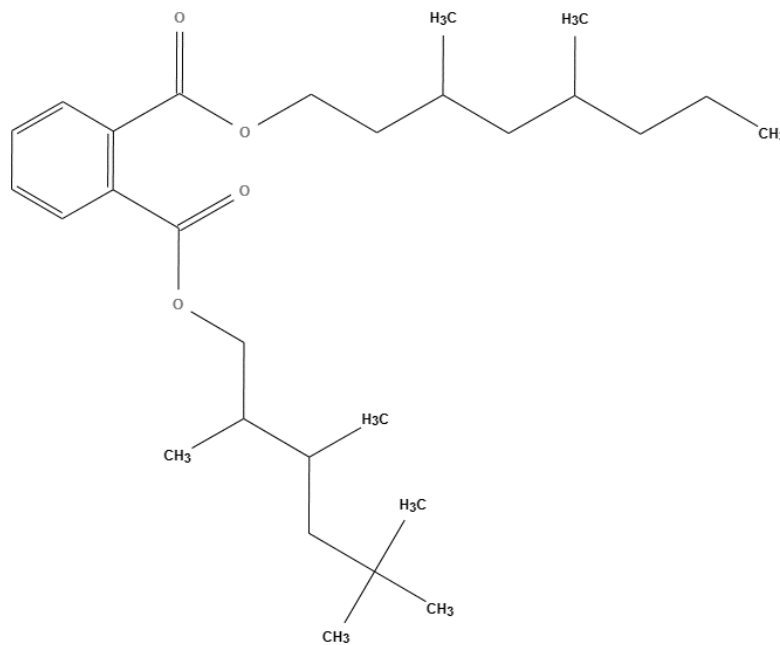


Draft Scope of the Risk Evaluation for Di- isodecyl Phthalate (DIDP)

Supplemental File:

Data Extraction and Data Evaluation Tables for Physical and Chemical Property Studies CASRNs 26761-40-0 and 68515-49-1



(Representative structure)

November 2020

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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 Di-Isodecyl Phthalate (DIDP)

Study Type	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	liquid		(NLM, 2015)	High

Table 2. Physical Properties Study Summary for DIDP

Study Type	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	clear liquid, mild odor		(NLM, 2015)	High
Experimental	colorless oily liquid with mild odor		(RSC, 2019)	High

Table 3. Melting Point Study Summary for DIDP

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	-50°C		(NLM, 2015)	High
Experimental	NR	-50°C		(RSC, 2019)	Medium
Experimental	NR	-50°C		(RSC, 2019)	Medium

Table 4. Boiling Point Study Summary for DIDP

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	250°C	These values are likely at reduced pressure (250-257°C at 4 mm Hg; PhysProp)	(RSC, 2019)	Medium
Experimental	NR	275°C	These values are likely at reduced pressure (250-257°C at 4 mm Hg; PhysProp)	(RSC, 2019)	Medium

Table 5. Density Study Summary for DIDP

Study Type	Study Details	Reference Substance	Temperature	Dynamic Viscosity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental			20°C		0.966 g/cm ³		(NLM, 2015)	High
Experimental			NR		0.965 g/cm ³		(RSC, 2019)	Medium
Experimental			293.15 K		0.9634 g/cm ³	Value at 298.15 K and 0.10 MPa; vibrating tube densimeter. The temperature was maintained within ±0.05 K, and the pressure had 0.11% uncertainty.	(Brito e Abreu et al., 2010)	High
Experimental			25°C		0.96283 g/cm ³	Determined with an Anton-Paar DMA5000 vibrating-tube densimeter; this source also measured pressure at 0.1 Mpa	(Harris and Bair, 2007)	High

Study Type	Study Details	Reference Substance	Temperature	Dynamic Viscosity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental			25°C		0.96285 g/cm ³	Value at 25°C and 0.1 MPa; determined with an Anton-Paar DMA5000 vibrating-tube densimeter; this source also measured density at atmospheric pressure	(Harris and Bair, 2007)	High
Experimental			25°C		0.96284 g/cm ³	Determined with an Anton-Paar DMA5000 vibrating-tube densimeter; this source also measured pressure at 0.1 MPa	(Harris and Bair, 2007)	High
Experimental			25°C		0.96284 g/cm ³	Value at 25°C and 0.1 MPa; determined with an Anton-Paar DMA5000 vibrating-tube densimeter; this source also measured density at atmospheric pressure	(Harris and Bair, 2007)	High
Experimental			NR		0.96284 g/cm ³	Reported as 962.84 kg/m ³ ; this source also measured densities up to 363.188 K	(Assael and Mylona, 2013)	High
Experimental			NR		0.96282 g/cm ³	Reported as 962.82 kg/m ³ ; estimated repeatability of (0.01%); measured using an automatic Anton Paar densimeter (model DMA 5000).	(Caetano et al., 2005)	High
Experimental			298.26 K		962.8 g/L	With 107 ppm water; reported as 962.8 kg/m ³	(Caetano et al., 2006)	High
Experimental			298.16 K		0.96290 g/cm ³	Value reported as 962.90 kg/m ³ at 298.16 K. Density measured via the vibrating tube method at atmospheric pressure, between 275.15 and 363.15 K.	(Froeba and Leipertz, 2007)	Medium
Experimental			293.15 K		0.9665 g/cm ³	Reported as 966.5 kg/m ³ at 293.15 K & 0.1 MPa pressure	(Peleties et al., 2010)	High

Study Type	Study Details	Reference Substance	Temperature	Dynamic Viscosity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental			298.15 K		0.9632 g/cm ³	298.15 K and 0.1 Mpa	(Paredes et al., 2009)	High
Experimental			298.15 K		0.9628 g/cm ³	298.15 K and 0.1 Mpa	(Paredes et al., 2009)	High
Experimental			298.15 K		0.9630 g/cm ³	298.15 K and 0.1 Mpa	(Paredes et al., 2009)	High
Experimental; Not Reported			298.15 K		0.9601 - 0.96461 g/cm ³	At pressure = 0.1MPa and T = 298.15K, density = 960.1 kg/m ³ +/- 2.9, viscosity = 87.5mPaS +/- 1.8 (Sample B). Sample A: density = 963.66 kg/m ³ (water mass fraction = 20E-6; viscosity = 87.2 mPa*s) Sample B: density = 960.1 kg/m ³ (water mass fraction = 417E-6; viscosity = 87.5 mPa*s) Sample C: density = 964.61 kg/m ³ (water mass fraction = 29E-6; viscosity 87.3 mPa*s)	(Al Motari et al., 2007)	High

Table 6. Vapor Pressure Study Summary for DIDP

Study Type	Substance Purity	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR		5.28E-7 mm Hg		(NLM, 2015)	High

Table 7. Vapor Density Study Summary for DIDP

No Vapor Density data was identified for this chemical.

Table 8. Water Solubility Study Summary for DIDP

Study Type	Substance Purity	Temperature	pH	Analytical Method	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	25°C	NR		0.28 mg/L		(NLM, 2015)	High
Experimental	Each sample contained less than 1 % of non-PAE material, as determined by another laboratory.	25°C	NR		1.19 mg/L	Water was ASTM Type 2 water	(Howard et al., 1985)	High

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

Study Type	Substance Purity	Temperature	pH	Other Study Details (Amounts of substance liquid phases)	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	NR	NR		10.352		(RSC, 2019)	High

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

No Henrys Law data was identified for this chemical.

Table 11. Flash Point Study Summary for DIDP

Study Type	Substance Purity	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR		232°C		(RSC, 2019)	Medium
Experimental	NR		122°C		(RSC, 2019)	Medium

Table 12. Auto Flammability Study Summary for DIDP

No Autoflammability data was identified for this chemical.

Table 13. Viscosity Study Summary for DIDP

Study Type	Apparatus	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental		20°C	108 cP		(NLM, 2015)	Medium
Experimental		298.25 K	87.67 cP	Reported as 87.67 mPa.s at 298.25 K, 0.1 MPa. Relative uncertainty was 0.8%	(Peleties and Trusler, 2011)	High
Experimental		25.1°C	88.70 cP	Reported as 88.70 mPa.s at 298.261 K; this source also measured viscosities up to 363.188 K	(Assael and Mylona, 2013)	High
Experimental		25°C	84.1 cP	0.1 MPa; The expanded uncertainty in the viscosity is estimated at 2%	(Harris and Bair, 2007)	High
Experimental		25°C	88.4 cP	0.1 MPa; The expanded uncertainty in the viscosity is estimated at 2%	(Harris and Bair, 2007)	High
Experimental		298.24 K	87.797 cP	The estimated overall uncertainty of the results does not exceed ±1%	(Caetano et al., 2005)	High
Experimental		298.22 K	86.72 cP	Reported as 86.72 mPa.s at 298.22 K	(Caetano et al., 2004)	High
Experimental		298.26 K	87.38 cP	Reported as 87.38 mPa.s	(Caetano et al., 2006)	High
Experimental; Not Reported		298.13 K	87.76 cP	298.13K = 87.76 mPa*S; 298.58K= 85.30 mPa*S	(da Mata et al., 2009)	High
Experimental; Not Reported		298.58 K	85.30 cP	298.13K, 87.76 mPa*S and 298.58K, 85.30 mPa*S	(da Mata et al., 2009)	High
Experimental; Not Reported		298.15K	87.2 cP	Sample A: 87.2 mPa*s (water mass fraction = 20E-6; density = 963.66 kg/m ³) Sample B: 87.5 mPa*s (water mass fraction = 417E-6; density = 960.1 kg/m ³) Sample C: 87.3 mPa*s (water mass fraction = 29E- 6; density = 964.61 kg/m ³)	(Al Motari et al., 2007)	High

Study Type	Apparatus	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Calculation		298.15 K	88.44 cP	Reported as 88.44mPa.S at atmospheric pressure calculated by dispersion relation; dispersion between liquid and gaseous phases are described by an equation which relates acceleration of gravity, dynamic viscosity, interfacial tension, and density. SLS was used to determine interfacial tension.	(Froebe and Leipertz, 2007)	High

Table 14. Refractive Index Study Summary for DIDP

Study Type	Apparatus	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental		1.483		(NLM, 2015)	High
Experimental	293.15 K	1.4845	Data consistent with the value supplied in the Merck Technical Data Sheet at the same temperature (1.485)	(Caetano et al., 2005)	High

Table 15. Dielectric Constant Study Summary for DIDP

No Dielectric Constant data was identified for this chemical.

EPI Suite™ Model Outputs

[\(U.S. EPA, 2012\)](#)

CAS Number: 26761-40-0

SMILES : CC(C)CCCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCC(C)C

CHEM : 1,2-Benzenedicarboxylic acid, diisodecyl ester

MOL FOR: C28 H46 O4

MOL WT : 446.68

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

Physical Property Inputs:

Log Kow (octanol-water): 10.35

Boiling Point (deg C) : -----

Melting Point (deg C) : -50.00

Vapor Pressure (mm Hg) : 5.28E-007

Water Solubility (mg/L): 0.28

Henry LC (atm-m3/mole) : -----

Log Octanol-Water Partition Coef (SRC):

Log Kow (KOWWIN v1.69 estimate) = 10.36

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

Boiling Pt (deg C): 463.36 (Adapted Stein & Brown method)

Melting Pt (deg C): 105.95 (Mean or Weighted MP)

VP(mm Hg,25 deg C): 2.29E-007 (Modified Grain method)

VP (Pa, 25 deg C) : 3.05E-005 (Modified Grain method)

MP (exp database): -50 deg C

BP (exp database): 250-257 @ 4 mm Hg deg C

VP (exp database): 5.28E-07 mm Hg (7.04E-005 Pa) at 25 deg C

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

Water Solubility at 25 deg C (mg/L): 1.006e-005

log Kow used: 10.35 (user entered)

melt pt used: -50.00 deg C

Water Sol (Exper. database match) = 0.28 mg/L (24 deg C)

Exper. Ref: YALKOWSKY,SH ET AL. (2010)

Water Sol Estimate from Fragments:

Wat Sol (v1.01 est) = 1.039e-005 mg/L

ECOSAR Class Program (ECOSAR v1.11):

Class(es) found:

Esters

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

Bond Method : 3.67E-005 atm-m3/mole (3.72E+000 Pa-m3/mole)

Group Method: 4.06E-005 atm-m3/mole (4.11E+000 Pa-m3/mole)

Exper Database: 1.11E-06 atm-m3/mole (1.12E-001 Pa-m3/mole)

For Henry LC Comparison Purposes:

User-Entered Henry LC: not entered

Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:

HLC: 1.108E-006 atm-m3/mole (1.123E-001 Pa-m3/mole)

VP: 5.28E-007 mm Hg (source: User-Entered)

WS: 0.28 mg/L (source: User-Entered)

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

Log Kow used: 10.35 (user entered)

Log Kaw used: -4.343 (exp database)

Log Koa (KOAWIN v1.10 estimate): 14.695

Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):

Biowin1 (Linear Model) : 0.8833

Biowin2 (Non-Linear Model) : 0.9920

Expert Survey Biodegradation Results:

Biowin3 (Ultimate Survey Model): 2.4925 (weeks-months)

Biowin4 (Primary Survey Model): 3.6612 (days-weeks)

MITI Biodegradation Probability:

Biowin5 (MITI Linear Model) : 0.7028

Biowin6 (MITI Non-Linear Model): 0.7039

Anaerobic Biodegradation Probability:

Biowin7 (Anaerobic Linear Model): 0.5119

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): 7.04E-005 Pa (5.28E-007 mm Hg)

Log Koa (Koawin est): 14.695

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

Mackay model : 0.0426

Octanol/air (Koa) model: 122

Fraction sorbed to airborne particulates (phi):

Junge-Pankow model : 0.606

Mackay model : 0.773

Octanol/air (Koa) model: 1

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

Hydroxyl Radicals Reaction:

OVERALL OH Rate Constant = 26.2168 E-12 cm³/molecule-sec

Half-Life = 0.408 Days (12-hr day; 1.5E6 OH/cm³)

Half-Life = 4.896 Hrs

Ozone Reaction:

No Ozone Reaction Estimation

Fraction sorbed to airborne particulates (phi):

0.69 (Junge-Pankow, Mackay avg)

1 (Koa method)

Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc : 1.099E+006 L/kg (MCI method)

Log Koc: 6.041 (MCI method)

Koc : 3.311E+006 L/kg (Kow method)

Log Koc: 6.520 (Kow method)

Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v2.00]:

Total Kb for pH > 8 at 25 deg C : 6.408E-002 L/mol-sec

Kb Half-Life at pH 8: 125.185 days

Kb Half-Life at pH 7: 3.427 years

(Total Kb applies only to esters, carbmates, alkyl halides)

Bioaccumulation Estimates (BCFBAF v3.01):

Log BCF from regression-based method = 1.885 (BCF = 76.74 L/kg wet-wt)

Log Biotransformation Half-life (HL) = 0.5524 days (HL = 3.568 days)

Log BCF Arnot-Gobas method (upper trophic) = 0.081 (BCF = 1.206)

Log BAF Arnot-Gobas method (upper trophic) = 0.950 (BAF = 8.903)

log Kow used: 10.35 (user entered)

Volatilization from Water:

Henry LC: 1.11E-006 atm-m³/mole (Henry experimental database)

Half-Life from Model River: 1117 hours (46.54 days)

Half-Life from Model Lake : 1.236E+004 hours (515.1 days)

Removal in Wastewater Treatment:

Total removal: 94.04 percent

Total biodegradation: 0.78 percent

Total sludge adsorption: 93.26 percent

Total to Air: 0.00 percent

(using 10000 hr Bio P,A,S)

Level III Fugacity Model: (MCI Method)

** Note: When the Log Kow is > 7, the model may be underestimating the mass of material in sediment and overestimating the mass of material in the water column (biota). Consider using the results of the default EQC model. **

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.27	9.79	1000
Water	15.7	900	1000
Soil	83.2	1.8e+003	1000
Sediment	0.912	8.1e+003	0
Persistence Time: 1.22e+003 hr			

Level III Fugacity Model: (MCI Method with Water percents)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.27	9.79	1000
Water	15.7	900	1000
water	(0.0139)		
biota	(15.6)		
suspended sediment	(0.0229)		
Soil	83.2	1.8e+003	1000
Sediment	0.912	8.1e+003	0
Persistence Time: 1.22e+003 hr			

Level III Fugacity Model: (EQC Default)

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
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Air	0.1	9.79	1000
Water	1.82	900	1000
water	(0.000122)		
biota	(0.137)		
suspended sediment	(1.69)		
Soil	30.9	1.8e+003	1000
Sediment	67.2	8.1e+003	0
Persistence Time:	3.3e+003	hr	

Data Evaluation Tables

Study Reference:	NLM. (2015)					
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical's physical/chemical properties.	1	1	1
Test Reliability	Reliability / Unbiased (Method Objectivity)	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Reliability / Analytical Method	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
Other	Databases	High	Data is from a publicly available and peer-reviewed database.	1	1	1
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Physical State reported by this reference.						
Cited reference: Lewis, R.J. Sr. 2007. Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY. P. 435.						

Study Reference: NLM. (2015)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
Test Reliability	Reliability / Unbiased (Method Objectivity)	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Reliability / Analytical Method	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
Other	Databases	High	Data is from a publicly available and peer-reviewed database.	1	1	1
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	2	2	2
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 rating for the Physical Properties reported by this reference.						
Cited reference: Lewis, R.J. Sr. 2007. Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY. P. 435.						

Study Reference: RSC. (2019)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
Test Reliability	Reliability / Unbiased (Method Objectivity)	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Reliability / Analytical Method	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
Other	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed original sources.	2	1	2
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	3	2	3
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 Physical Properties reported by this reference.						
Cited reference: Oxford University Chemical Safety Data						

Study Reference: NLM. (2015)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical'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 publicly available, peer-reviewed database that provides references to a recognized data collection.	1	1	1
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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: Haynes, W.M. (Ed.) 2014. CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014. p. 3-194.

Study Reference: RSC. (2019)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	Medium	Data are measured or estimated for the subject chemical substance.	2	1	2
	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	Low	The analytical method is unknown and there is no indication that a reliable method was used	3	1	3
Other	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.	2	1	2
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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):	2
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Medium
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. (2019)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical'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	Low	The analytical method is unknown and there is no indication that a reliable method was used	3	1	3
Other	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.	2	1	2
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	9	5	9
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.8	Overall Score (Rounded):	1.8
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Medium

The reviewer agreed with the overall rating for the Melting Point reported by this reference.
Cited reference: Oxford University Chemical Safety Data

Study Reference: RSC. (2019)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical'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	Low	The analytical method is unknown and there is no indication that a reliable method was used	3	1	3
Other	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.	2	1	2
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	9	5	9
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.8	Overall Score (Rounded):	1.8
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Medium
The reviewer agreed with the overall rating for the Boiling Point reported by this reference. Cited reference: Matrix Scientific						

Study Reference: RSC. (2019)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical'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	Low	The analytical method is unknown and there is no indication that a reliable method was used	3	1	3
Other	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.	2	1	2
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	9	5	9
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.8	Overall Score (Rounded):	1.8
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Medium

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

Cited reference: Oxford University Chemical Safety Data

Study Reference: Caetano et al. (2006).						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: Brito e Abreu, et al. (2010)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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	Medium	The analytical method is non-standard but is expected to be appropriate.	2	1	2
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	4	3	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.33	Overall Score (Rounded):	1.33
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference: Assael and Mylona. (2013)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: Harris, KR; Bair, S. (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: Harris, KR; Bair, S. (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: Harris, KR; Bair, S. (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: Harris, KR; Bair, S. (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: Caetano, et al. (2005)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: Froeba and Leipertz (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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. Methodology well described, supporting theory lacking characterization.	2	1	2
	Reliability / Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate. Analytical method appears to be common, but no standard method is stated.	2	1	2
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	5	3	5
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.67	Overall Score (Rounded):	1.67
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Medium

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

Study Reference: Peleties et al. (2010)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: Paredes et al. (2009)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: Paredes et al. (2009)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: Paredes et al. (2009)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: AI Motari et al. (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Density reported by this reference.

Study Reference: NLM. (2015)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 publicly available, peer-reviewed database that provides references to a peer-reviewed data collection.	1	1	1
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer agreed with the overall rating for the Density reported by this reference.						
Cited reference: Haynes, W.M. (Ed.) 2014. CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL 2014. p. 3-194.						

Study Reference: RSC. (2019)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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	Low	The analytical method is unknown and there is no indication that a reliable method was used.	3	1	3
Other	Databases	Medium	Data is from a secondary database with references to the peer-reviewed original source.	2	1	2
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	8	4	8
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	2	Overall Score (Rounded):	2
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Medium
The reviewer agreed with the overall rating for the Density reported by this reference. Cited reference: Matrix Scientific						

Study Reference: NLM. (2015)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical'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 publicly available, peer-reviewed database that provides references to original sources.	1	1	1
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 Vapor Pressure reported by this reference.

Cited reference: Yaws, C.L. 1994. Handbook of Vapor Pressure, Vol 3 C8 to C28, Houston, TX: Gulf Publishing Co.

Study Reference: NLM. (2015)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical'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 publicly available database that provides references to original sources.	1	1	1
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer agreed with the overall rating for the Water Solubility reported by this reference.						
Cited reference: Yalkowsky, S.H., He, Yan, Jain, P. 2010. Handbook of Aqueous Solubility Data Second Edition. CRC Press, Boca Raton, FL. P. 1325.						

Study Reference: Howard et al. (1985)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) and other physical/chemical properties	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Water Solubility reported by this reference.

Study Reference: RSC. (2019)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	High	Measured data are consistent with the subject chemical'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 publicly available secondary source with references to non-peer reviewed sources.	1	1	1
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	7	5	7
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.4	Overall Score (Rounded):	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference: RSC. (2019)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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	Low	The analytical method is unknown and there is no indication that a reliable method was used	3	1	3
Other	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.	2	1	2
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	8	4	8
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	2	Overall Score (Rounded):	2
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Medium
The reviewer agreed with the overall rating for the Flash Point reported by this reference. Cited reference: LabNetwork						

Study Reference: RSC. (2019)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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	Low	The analytical method is unknown and there is no indication that a reliable method was used	3	1	3
Other	Databases	Medium	Data is from a publicly available secondary source with references to non-peer reviewed sources.	2	1	2
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	8	4	8
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	2	Overall Score (Rounded):	2
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	Medium

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

Cited reference: Oxford University Chemical Safety Data

Study Reference: Caetano et al. (2006).						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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	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	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	4	3	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.33	Overall Score (Rounded):	1.33
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference: Peleties and Trusler (2011)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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. Methodology and theory were well characterized.	1	1	1
	Reliability / Analytical Method	Medium	The analytical method is non-standard but is expected to be appropriate. The analytical method did not follow a stated standard.	2	1	2
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	4	3	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.33	Overall Score (Rounded):	1.33
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference: Froeba and Leipertz (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information	NR	1	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	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	High	The model had a defined, unambiguous endpoint AND the model performance was known and $r^2 > 0.7$, $q^2 > 0.5$, and $SE < 0.3$ (ECHA, 2016).	1	1	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 rating for the Viscosity reported by this reference.

Study Reference: Froeba and Leipertz (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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	Medium	The analytical method is non-standard but is expected to be appropriate.	2	1	2
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	4	3	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.33	Overall Score (Rounded):	1.33
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High
The reviewer agreed with the overall rating for the Viscosity reported by this reference.						
Study Reference: Assael and Mylona. (2013)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1

	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Viscosity reported by this reference.						

Study Reference: Harris, KR; Bair, S. (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Viscosity reported by this reference.

Study Reference: Harris, KR; Bair, S. (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Viscosity reported by this reference.

Study Reference: Caetano, et al. (2005)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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	Medium	Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard.	2	1	2
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	4	3	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.33	Overall Score (Rounded):	1.33
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference: Caetano et al. (2004)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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	Medium	The analytical method is non-standard but is expected to be appropriate.	2	1	2
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	4	3	4
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.33	Overall Score (Rounded):	1.33
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

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

Study Reference: da Mata et al. (2009)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Viscosity reported by this reference.

Study Reference: da Mata et al. (2009)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Viscosity reported by this reference.

Study Reference: AI Motari et al. (2007)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Viscosity reported by this reference.

Study Reference: NLM. (2015)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 publicly available, peer-reviewed database that provides references to a recognized data collection.	1	1	1
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
			Sum of scores:	6	4	6
High	Medium	Low	Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:	1.5	Overall Score (Rounded):	1.5
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			Overall Quality Level:	High

The reviewer agreed with the overall rating for the Viscosity reported by this reference.
Cited reference: Lewis, R.J. Sr. 2007. Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY. P. 435.

Study Reference: Caetano, et al. (2005)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 other developed standard.	1	1	1
Other	Databases	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	NR
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 rating for the Refractive Index reported by this reference.

Study Reference: NLM. (2015)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	High	Data are measured or estimated for the subject chemical substance.	1	1	1
	Appropriateness	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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 publicly available, peer-reviewed database that provides references to a recognized data collection.	1	1	1
	Models	Not rated	Rating of this factor is not applicable to this kind of information.	NR	1	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: Lewis, R.J. Sr. 2007. Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY. P. 435.						

Study Reference: U.S. EPA (2012)						
Domain	Metric	Qualitative Determination [i.e., High, Medium, Low, Unacceptable, or Not rated]	Comments	Metric Score	Metric Weighting Factor	Weighted Score
Substance	Representativeness	Not rated	The metric is not applicable to this study type (SAR).	NR	1	NR
	Appropriateness	Not rated	The metric is not applicable to this study type (SAR).	NR	1	NR
Test Reliability	Reliability / Unbiased (Method Objectivity)	Not rated	The metric is not applicable to this study type (SAR).	NR	1	NR
	Reliability / Analytical Method	Not rated	The metric is not applicable to this study type (SAR).	NR	1	NR
Other	Databases	Not rated	The metric is not applicable to this study type (SAR).	NR	1	NR
	Models	High	The models in EPI Suite™ have defined endpoints. Chemical domain and performance statistics for each model are known, and unambiguous algorithms are available in the EPI Suite™ documentation and/or cited references to establish their scientific validity. Many EPI Suite™ models have correlation coefficients >0.7, cross-validated correlation coefficients >0.5, and standard error values <0.3; however, correlation coefficients (r^2 , q^2) for the regressions of some environmental fate models (i.e., BIOWIN) are lower, as expected, compared to regressions which	1	1	1

			have specific experimental values such as water solubility or log Kow (octanol-water partition coefficient).			
			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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