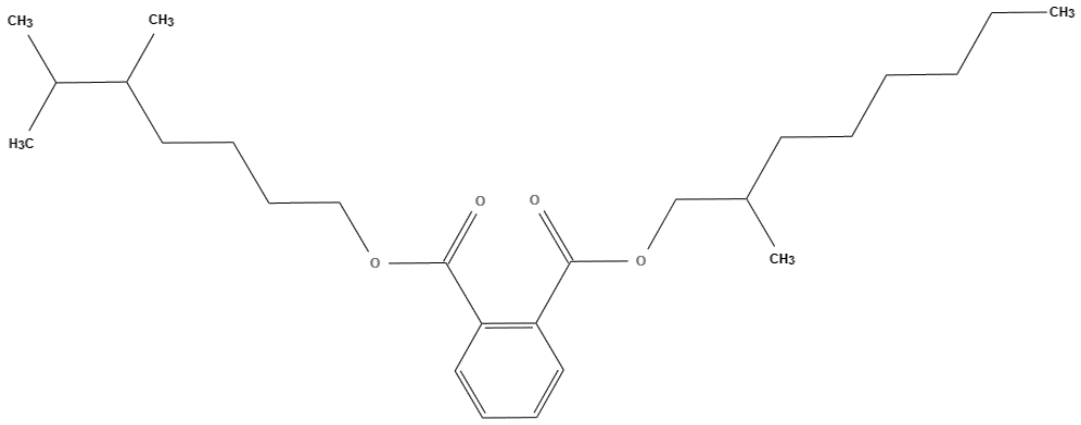
United States
Environmental Protection Agency

Office of Chemical Safety and
Pollution Prevention

Draft Scope of the Risk Evaluation for Di-isononyl Phthalate (DINP)

Supplemental File:

Data Extraction and Data Evaluation Tables for Physical and Chemical Property Studies CASRN: 28553-12-0 and 68515-48-0



(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-Isononyl Phthalate

Study Type	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	**liquid**		**(NLM, 2015)**	**High**
Experimental	liquid		(O'Neil, 2013)	High

Table 2. Physical Properties Study Summary for Di-Isononyl Phthalate

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

Table 3. Melting Point Study Summary for Di-Isononyl Phthalate

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	**NR**	**-48°C**		**(NLM, 2015)**	**High**
Experimental	NR	-48°C		(O'Neil, 2013)	High

Table 4. Boiling Point Study Summary for Di-Isononyl Phthalate

Study Type	Substance Purity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	**NR**	**252°C**	**at 5 torr**	**(O'Neil, 2013)**	**High**

Table 5. Density Study Summary for Di-Isononyl Phthalate

Study Type	Study Details	Reference Substance	Temperature	Dynamic Viscosity	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental			20°C		0.972 g/cm^3	at 20°C relative to water at 20°C	(O'Neil, 2013)	High
Experimental					0.972 g/cm^3		(NLM, 2015)	High
Experimental			**293.15 K**		**0.97578 g/cm^3**	**Interpolated value at 293.15 K. Value derived from measurements taken between 287.90 through 366.12 K. Density experimental data (g/cm^3): 0.97943 at 287.90 K, 0.97187 at 298.15 K, 0.96607 at 308.22 K, 0.95739 at 318.20 K, 0.95003 at 328.17 K, 0.94308 at 338.44 K, 0.93674 at 348.01 K, 0.92889 at 358.91 K, 0.92396 at 366.12 K.**	**(De Lorenzi et al., 1998)**	**High**

Table 6. Vapor Pressure Study Summary for Di-Isononyl Phthalate

Study Type	Substance Purity	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	100°C	0.0018 mm Hg		(O'Neil, 2013)	High
Experimental	NR	200°C	0.50 mm Hg		(O'Neil, 2013)	High
Experimental	NR	300°C	40 mm Hg		(O'Neil, 2013)	High
Experimental	NR	25°C	5.4E-7 mm Hg		(NLM, 2015)	High
Experimental	**Each sample contained less than 1% of non-PAE material, as determined by another laboratory.**	**25°C**	**5.4E-7 mm Hg**	**Value reported as 7.5E-5 Pa**	**(Howard et al., 1985)**	**High**

Table 7. Vapor Density Study Summary for Di-Isononyl Phthalate

No Vapor Density data was identified for this chemical.

Table 8. Water Solubility Study Summary for Di-Isononyl Phthalate

Study Type	Substance Purity	Temperature	pH	Analytical Method	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental	NR	20°C	NR		0.2 mg/L		(NLM, 2015)	High
Experimental	**Each sample contained less than 1% of non-PAE material, as determined by another laboratory.**	**25°C**	**NR**		**0.2 mg/L**	**water was ASTM Type 2 water**	**(Howard et al., 1985)**	**High**

Table 9. Octanol Water Coefficient (logKow) Study Summary for Di-Isononyl Phthalate

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		9.37		(O'Neil, 2013)	High
Experimental	**NR**	**NR**	**NR**		**9.37**		**(NLM, 2015)**	**High**

Table 10. Henry's Law Constant Study Summary for Di-Isononyl Phthalate

No Henrys Law data was identified for this chemical.

Table 11. Flash Point Study Summary for Di-Isononyl Phthalate

Study Type	Substance Purity	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental; closed cup	**NR**	**213°C (415°F)**	**213°C**		**(O'Neil, 2013)**	High

Table 12. Auto Flammability Study Summary for Di-Isononyl Phthalate

No Auto flammability data was identified for this chemical.

Table 13. Viscosity Study Summary for Di-Isononyl Phthalate

Study Type	Apparatus	Temperature	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental		20°C		102 cST; kinematic viscosity	(NLM, 2015)	High
Experimental		**298.15 K**	**55.334 cP**	**Experimental viscosity data (mPa*s): 101.95 at 291.29 K, 55.334 at 298.15 K, 32.812 at 308.17 K, 21.035 at 319.06 K, 13.812 at 327.98 K, 9.9061 at 337.87 K, 7.3961 at 348.72 K, 5.7089 at 358.64 K, and 4.5214 at 368.49 K.**	**(De Lorenzi et al., 1998)**	**High**

Table 14. Refractive Index Study Summary for Di-Isononyl Phthalate

Study Type	Apparatus	Result	Comments	Affiliated Reference	Data Quality Evaluation Results
Experimental		1.486		(O'Neil, 2013)	High
Experimental		1.486		(NLM, 2015)	High
Experimental	**293.15 K**	**1.48610**	**Value interpolated at 293.15 K. Experimental refractive index data: 1.4883 at 288.15 K, 1.4860 at 294.35 K, 1.4846 at 298.15 K, 1.4828 at 302.75 K, 1.4809 at 307.95 K, 1.4788 at 313.35 K, 1.4769 at 318.15 K, and 1.4753 at 322.25 K.**	**(De Lorenzi et al., 1998)**	**High**
Experimental	24	1.524	The reference signal is a THz pulse transmitted through the empty crystal cell with a correction applied to account for the effect of the crystal cell absorbing THz waves. The experimental result is entered into a mathematical equation to calculate the refractive index.	(Liu et al., 2016)	High

Table 15. Dielectric Constant Study Summary for Di-Isononyl Phthalate

No Dielectric Constant data was identified for this chemical.

EPI Suite™ Model Outputs

(U.S. EPA, 2012)

SMILES : O=C(c1ccccc1C(=O)OCCCCCCCC(C)C)OCCCCCCCC(C)C
CHEM :
MOL FOR: C26 H42 O4
MOL WT : 418.62
---------- EPI SUMMARY (v4.11) ----------
Physical Property Inputs:
Log Kow (octanol-water): 9.37
Boiling Point (deg C) : ------
Melting Point (deg C) : -48.00
Vapor Pressure (mm Hg) : 5.4E-007
Water Solubility (mg/L): 0.2
Henry LC (atm-m3/mole) : ------

Log Octanol-Water Partition Coef (SRC):
Log Kow (KOWWIN v1.68 estimate) = 9.37

Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPVP v1.43):
Boiling Pt (deg C): 440.16 (Adapted Stein & Brown method)
Melting Pt (deg C): 84.91 (Mean or Weighted MP)
VP(mm Hg,25 deg C): 8.62E-007 (Modified Grain method)
VP (Pa, 25 deg C) : 0.000115 (Modified Grain method)
VP (exp database): 5.40E-07 mm Hg (7.20E-005 Pa) at 25 deg C

Water Solubility Estimate from Log Kow (WSKOW v1.42):
Water Solubility at 25 deg C (mg/L): 0.0001012
log Kow used: 9.37 (user entered)
melt pt used: -48.00 deg C
Water Sol (Exper. database match) = 0.2 mg/L (20 deg C)
Exper. Ref: HOWARD,PH ET AL. (1985)

Water Sol Estimate from Fragments:
Wat Sol (v1.01 est) = 0.00011547 mg/L

ECOSAR Class Program (ECOSAR v1.11):
Class(es) found:
Esters

Henrys Law Constant (25 deg C) [HENRYWIN v3.20]:
Bond Method : 2.08E-005 atm-m3/mole (2.11E+000 Pa-m3/mole)
Group Method: 2.03E-005 atm-m3/mole (2.06E+000 Pa-m3/mole)
Exper Database: 1.49E-06 atm-m3/mole (1.51E-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: 1.487E-006 atm-m3/mole (1.507E-001 Pa-m3/mole)

VP: 5.4E-007 mm Hg (source: User-Entered)
WS: 0.2 mg/L (source: User-Entered)

Log Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1.10]:
Log Kow used: 9.37 (user entered)
Log Kaw used: -4.215 (exp database)
Log Koa (KOAWIN v1.10 estimate): 13.585
Log Koa (experimental database): None

Probability of Rapid Biodegradation (BIOWIN v4.10):
Biowin1 (Linear Model) : 0.8966
Biowin2 (Non-Linear Model) : 0.9946
Expert Survey Biodegradation Results:
Biowin3 (Ultimate Survey Model): 2.5545 (weeks-months)
Biowin4 (Primary Survey Model) : 3.7017 (days-weeks)
MITI Biodegradation Probability:
Biowin5 (MITI Linear Model) : 0.6804
Biowin6 (MITI Non-Linear Model): 0.6996
Anaerobic Biodegradation Probability:
Biowin7 (Anaerobic Linear Model): 0.4600
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): 7.2E-005 Pa (5.4E-007 mm Hg)
Log Koa (Koawin est): 13.585
Kp (particle/gas partition coef. (m3/ug)):
Mackay model : 0.0417
Octanol/air (Koa) model: 9.44
Fraction sorbed to airborne particulates (phi):
Junge-Pankow model : 0.601
Mackay model : 0.769
Octanol/air (Koa) model: 0.999

Atmospheric Oxidation (25 deg C) [AopWin v1.92]:
Hydroxyl Radicals Reaction:
OVERALL OH Rate Constant = 23.3907 E-12 cm3/molecule-sec
Half-Life = 0.457 Days (12-hr day; 1.5E6 OH/cm3)
Half-Life = 5.487 Hrs
Ozone Reaction:
No Ozone Reaction Estimation
Fraction sorbed to airborne particulates (phi):
0.685 (Junge-Pankow, Mackay avg)
0.999 (Koa method)
Note: the sorbed fraction may be resistant to atmospheric oxidation

Soil Adsorption Coefficient (KOCWIN v2.00):

Koc : 3.309E+005 L/kg (MCI method)
Log Koc: 5.520 (MCI method)
Koc : 9.479E+005 L/kg (Kow method)
Log Koc: 5.977 (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 = 2.366 (BCF = 232.4 L/kg wet-wt)
Log Biotransformation Half-life (HL) = 0.2742 days (HL = 1.88 days)
Log BCF Arnot-Gobas method (upper trophic) = 0.394 (BCF = 2.479)
Log BAF Arnot-Gobas method (upper trophic) = 1.142 (BAF = 13.88)
log Kow used: 9.37 (user entered)

Volatilization from Water:
Henry LC: 1.49E-006 atm-m3/mole (Henry experimental database)
Half-Life from Model River: 806.1 hours (33.59 days)
Half-Life from Model Lake : 8965 hours (373.5 days)

Removal in Wastewater Treatment:
Total removal: 94.03 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:

	Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)
Air	0.286	11	1000
Water	15.2	900	1000
Soil	82	1.8e+003	1000
Sediment	2.53	8.1e+003	0

Persistence Time: 1.25e+003 hr

Data Evaluation Tables

Study Reference:	O'Neil (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	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 recognized data collection where data are peer- reviewed by experts in the field.	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.						

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: Haynes, W.M. (Ed.) 2014. CRC Handbook of Chemistry and Physics. CRC Press LLC, Boca Raton: FL 2014. p. 3-194.						

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: Haynes, W.M. (Ed.) 2014. CRC Handbook of Chemistry and Physics. CRC Press LLC, Boca Raton: FL 2014. p. 3-194.						

Study Reference:	O'Neil (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	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/recognize d database or other secondary source.	2	1	2
Other	**Databases**	High	Data is from a recognized, 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:	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: O'Neil, M.J. (Ed.). 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. p. 598-599.						

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/recognize d 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: O'Neil, M.J. (Ed.) 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. P. 598						

Study Reference:	O'Neil (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	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/recognize d database or other secondary source.	2	1	2
Other	**Databases**	High	Data is from a recognized, 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:	7	5	7
High	Medium	Low	**Overall Score = Sum of Weighted Scores/Sum of Metric Weighting Factors:**	1.4	**Overall Score (Rounded):**	1.4
≥1 and <1.7	≥1.7 and <2.3	≥2.3 and ≤3			**Overall Quality Level:**	High
The reviewer agreed with the overall rating for the Boiling Point reported by this reference.						
Cited reference: O'Neil, M.J. (Ed.). 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. p. 598-599.						

Study Reference:	De Lorenzi et al., 1998					
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:	O'Neil (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)**	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/recognize d database or other secondary source.	2	1	2
Other	**Databases**	High	Data is from a recognized, 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.						

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/recognize d 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: O'Neil, M.J. (Ed.) 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. P. 598						

Study Reference:	O'Neil (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	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/recognize d database or other secondary source.	2	1	2
Other	**Databases**	High	Data is from 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:	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: O'Neil, M.J. (Ed.). 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. p. 598-599.						

Study Reference:	O'Neil (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	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/recognize d database or other secondary source.	2	1	2
Other	**Databases**	High	Data is from 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:	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: O'Neil, M.J. (Ed.). 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. p. 598-599.						

Study Reference:	O'Neil (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	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/recognize d database or other secondary source.	2	1	2
Other	**Databases**	High	Data is from 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:	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: O'Neil, M.J. (Ed.). 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. p. 598-599.						

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/recognize d 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: Howard, P.H. et al. 1985. Environ Toxicol Chem 4: 653-61						

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 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	standard method reported in peer-reviewed journal	1	1	1
	Reliability / Analytical Method	High	standard method with experimental details	1	1	1
Other	**Databases**	Not rated	Not applicable	NR	1	NR
	Models	Not rated	Not applicable	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 Vapor Pressure 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	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/recognize d 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: Howard, P.H. et al. 1985. Environ Toxicol Chem 4: 653-61						

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	Standard test method	1	1	1
	Reliability / Analytical Method	High	Protocol was designed to meet or exceed the requirements of the EPA-recommended procedure	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:	O'Neil (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	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/recognize d database or other secondary source.	2	1	2
Other	**Databases**	High	Data is from a recognized, 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:	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: O'Neil, M.J. (Ed.). 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. p. 598-599.						

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/recognize d database or other secondary source.	2	1	2
Other	**Databases**	High	Data is from a publicly available database that provides references to a peer-reviewed source.	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: O'Neil, M.J. (Ed.) 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. P. 598						

Study Reference:	O'Neil (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)**	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/recognize d database or other secondary source.	2	1	2
Other	**Databases**	High	Data is from a recognized, 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 Flash Point reported by this reference.						

Study Reference:	De Lorenzi et al. (1998)					
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:	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/recognize d 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: O'Neil, M.J. (Ed.) 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. P. 598						

Study Reference:	De Lorenzi et al. (1998)					
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 Refractive Index reported by this reference.						

Study Reference:	Liu et al. (2016)					
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 was 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	Methodology clearly stated.	1	1	1
	Reliability / Analytical Method	High	Experimental procedures and analytical methods were clearly delineated.	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:	O'Neil (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)**	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/recognize d database or other secondary source.	2	1	2
Other	**Databases**	High	Data is from a recognized, 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 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/recognize d 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: O'Neil, M.J. (Ed.) 2013. The Merck Index - An Encyclopedia of Chemicals, Drugs, and Biologicals. Cambridge, UK: Royal Society of Chemistry. P. 598						

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	1	1	1

			regressions which 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

References

De Lorenzi, L; Fermeglia, M; Torriano, G. (1998). Density, kinematic viscosity, and refractive index for bis(2-ethylhexyl) adipate, tris(2-ethylhexyl) trimellitate, and diisononyl phthalate. Journal of Chemical and Engineering Data 43: 183-186. http://dx.doi.org/10.1021/je970200z

Howard, PH; Banerjee, S; Robillard, KH. (1985). Measurement of water solubilities octanol-water partition coefficients and vapor pressures of commercial phthalate esters. Environ Toxicol Chem 4: 653-662. http://dx.doi.org/10.1002/etc.5620040509

Liu, L; Shen, L; Yang, F; Han, F; Hu, P; Song, M. (2016). Determining Phthalic Acid Esters Using Terahertz Time Domain Spectroscopy. Journal of Applied Spectroscopy 83: 603-609. http://dx.doi.org/10.1007/s10812-016-0335-9

NLM (National Institutes of Health, National Library of Medicine). (2015). PubChem: Hazardous Substance Data Bank: Di-isononyl phthalate, 28553-12-0. Available online at https://pubchem.ncbi.nlm.nih.gov/compound/590836#source=HSDB

O'Neil, MJ. (2013). Diisononyl phthalate. In The Merck index (15th ed.). Cambridge, UK: Royal Society of Chemistry.

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