Draft Physical Chemistry, Fate, and Transport Assessment for Dicyclohexyl Phthalate (DCHP)

Technical Support Document for the Draft Risk Evaluation

CASRN 84-61-7

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127	DCHP	Dicyclohexyl phthalate	
128	EC50	Effect concentration at which 50 percent of test organisms exhibit an effect	
129	ECHA	European Chemicals Agency	
130	LC50	Lethal concentration at which 50 percent of test organisms die	
131	NITE	National Institute of Technology and Evaluation	
132	OCSPP	Office of Chemical Safety and Pollution Prevention	
133	OECD	Organisation for Economic Co-operation and Development	
134	OPPT	Office of Pollution Prevention and Toxics	
135	QSPR	Quantitative structure property relationship models	
136	TSCA	Toxic Substances Control Act	
137			

SUMMARY

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- This technical document is in support of the Toxic Substances Control Act (TSCA) *Draft Risk*
- 140 Evaluation for Dicyclohexyl Phthalate (DCHP) (U.S. EPA, 2024d). DCHP is a common chemical name
- 141 for the chemical substance dicyclohexyl phthalate (CASRN 84-61-7). See the draft risk evaluation for a
- complete list of all the technical support documents for DCHP.

DCHP – Chemistry, Fate, and Transport: Key Points

EPA evaluated the reasonably available information to characterize the physical-chemical and environmental fate and transport of DCHP. The key points are summarized below. DCHP

- is a granular, crystalline solid under environmental conditions (Section 2.4.1);
- has a tendency to partition to soil, sediment, and particulate over water or air when released to air and later deposited (Sections 2.4.9, 2.4.10, and 2.4.13);
- has limited solubility in water (Sections 2.4.8); and
- has low volatility in water or soil (Section 2.4.12 and 2.4.11).

Given the consistent results from numerous high-quality studies, there is robust evidence that when present in the environment, DCHP

- may degrade through hydrolysis (Section 3.2.1), photolysis (Section 3.2.2), aerobic or anaerobic biodegradation (Section 3.2.3);
- may transport through the air and be deposited to soil or water (Section 3.4.1);
- will sorb to particulate in the atmosphere (Sections 3.4.1.1 and 3.4.1.2) and in water (Sections 3.4.2.2 and 3.4.3.1); and
- is expected to be removed in wastewater treatment processes by sorbing to particulate, biosolids, and sludge (Section 3.5.2).

As a result of limited studies identified, there is moderate confidence that DCHP

- may be partially removed in conventional drinking water treatment (Section 3.5.3); and
- may accumulate in individual fish and aquatic organisms but is not expected to move up the food chain in aquatic environments (Section 3.6).

EPA considered all reasonably available information identified by the systematic review process under TSCA to characterize the chemistry and fate and transport of DCHP. When experimental values were not available, EPI SuiteTM and empirical models were used to estimate values.

The following bullets summarize the key points of the partitioning analysis (Section 3.3). DCHP

- will remain mostly in water but may sorb to sediment when released to aquatic environments;
- will sorb to atmospheric particulate but may end up in small amounts in soil, water, and sediment when released to air;
- will remain exclusively in soil when released to soil;
- will sorb to particulate phases (soil, sediment, air particulate) with a small amount ending up in water when released to all three phases (air, water, and soil).

1 INTRODUCTION

EPA is evaluating the health and environmental risks of dicyclohexyl phthalate (DCHP) under TSCA)

DCHP is a medium-chained branched phthalate ester with the chemical equation C₂₀H₂₆O₄ and a molar mass of 330.43 g/mol (EC/HC, 2017). It is solid at room temperature with a water solubility equal to or less than 1.48 mg/L (EC/HC, 2017). DCHP has a melting point of 66 °C, boiling point of 225 °C (4 mm hg), and Henry's Law coefficient (constant) of 9.446×10⁻⁸ atm-m³/mol and has been categorized as a non-volatile organic compound (NVOC) (EC/HC, 2017).

DCHP is produced by the esterification of phthalic anhydride with cyclohexanols. Typical technical grade DCHP has a purity of at least 99.0 percent (by ester content) with 0.1 percent maximum moisture content and 0.15 percent acidity (as phthalic acid) (CPSC, 2011). DCHP, either alone or in combination with other phthalates, is commonly used as a plasticizer in the production of plastics and other polymers, in sealants and adhesives for paper food packaging, and as a preservation agent in peroxides (CPSC, 2011).

Environmental release data for DCHP were not available from the Toxics Release Inventory (TRI) or through Discharge Monitoring Reports (DMRs). However, between 500,000 and 1,000,000 pounds (lb) of DCHP were produced annually from 2016 to 2019 for use in commercial products, chemical substances or mixtures sold to consumers, or at industrial sites nationwide according to production data from the Chemical Data Reporting (CDR) 2020 reporting period. These production volumes suggest that DCHP may have releases from fugitive or stack air emissions, releases to water, and releases to landfills during production, distribution, processing in poly vinyl chloride and non-PVC polymers, use of products such as paints and sealants, disposal or recycling, wastewater treatment, and disposal of solid and liquid waste (ECJRC, 2003b).

The following sections of this draft TSD discuss the selection of the physical properties, chemical properties, and environmental fate of DCHP in the environment.

2 PHYSICAL AND CHEMICAL PROPERTY ASSESSMENT OF DCHP

2.1 Approach and Methodology

EPA gathered and evaluated physical and chemical property data and information according to the process described in the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances, Version 1.0: A Generic TSCA Systematic Review Protocol with Chemical-Specific Methodologies* (also called the "2021 Draft Systematic Review Protocol") (<u>U.S. EPA, 2021</u>). During the evaluation of DCHP, EPA considered both measured and estimated physical and chemical property data/information summarized in Table 2-1, as applicable. Information on the full, extracted dataset is

data/information summarized in Table 2-1, as applicable. Information on the full, extracted data available in the supplemental file *Draft Risk Evaluation for Dicyclohexyl Phthalate (DCHP)* –

181 Systematic Review Supplemental File: Data Quality Evaluation and Data Extraction Information for

Physical and Chemical Properties (U.S. EPA, 2024b).

2.2 Evidence Integration for Physical and Chemical Properties

Only sources with an overall data quality ranking of high or medium were selected for use in determining the representative physical and chemical properties of DCHP for the purposes of the risk evaluation. The Environment and Climate Change Canada Phthalate Substance Group Screening Assessment and *ECHA State of the Science Report on Medium-Chain Phthalate Ester* were evaluated to consider how the findings from the present analysis compared to international assessments (EC/HC, 2017). The surveyed high-quality sources typically agree with the selected value or selected range of values provided in the EC/HC (2017) document.

When data were not available for a specific parameter or there is uncertainty associated with the reported value(s) EPA used models as noted to estimate specific parameters. EPI SuiteTM estimated parameters were selected as the representative value for the following physical and chemical parameters: water solubility (WATERNT and WSKOW), K_{OA} (KOAWIN), and Henry's Law constant (HENRYWIN).

2.3 Selected Physical and Chemical Property Values for DCHP

The selected physical and chemical property values for DCHP are provided in Table 2-1 and discussed in Section 3.4. Results of values that were modeled in EPI SuiteTM are provided in 0.

Table 2-1. Final Selected Physical and Chemical Property Values for DCHP

Property	Selected Value Reference		Overall Quality Determination
Molecular formula	$C_{20}H_{26}O_4$		
Molecular weight	330.43 g/mol		
Physical form	Solid, prism	(<u>Haynes</u> , 2014)	High
Physical properties	White granular solid	(NLM, 2024b)	High
Melting point	66 °C	(Haynes, 2014)	High
Boiling point	225 °C at 4 mm Hg	(Haynes, 2014)	High
Density	1.383 g/cm ³	(Haynes, 2014)	High
Vapor Pressure	8.69E-7 mmHg	(NLM, 2024b)	High

Property	Selected Value	Reference	Overall Quality Determination
Vapor Density	No Data		
Water Solubility	0.030–1.48 mg/L ^a	(U.S. EPA, 2017)	Medium
Octanol:Water partition coefficient (log KOW)	4.82	(EC/HC, 2017)	High
Octanol:Air Partition Coefficient (log K _{OA})	10.23 ^a	(U.S. EPA, 2017)	Medium
Henry's Law Constant	9.446E–8 atm·m³/mol ^a at 25 °C	(U.S. EPA, 2017)	Medium
Flash Point	207 °C	(RSC, 2019a)	Medium
Auto-Flammability	No data		
Viscosity	Solid, N/A	(NLM, 2024b)	High
^a Modeled value using EPI	Suite TM		

2.4 Endpoint Assessments

2.4.1 Physical Form and Properties

EPA extracted and evaluated three high-quality sources containing information regarding the physical form of DCHP. All three sources reported that DCHP was solid under standard temperature and pressure (25 °C, 1 atm) with a white, granular, prismatic solid form (NLM, 2024b; Haz-Map, 2022; Haynes, 2014). Thus a solid state was selected as the representative state of matter for DCHP under environmental conditions. The selected state of matter is consistent with the selected values for DCHP's boiling point (225 °C) and melting point (66 °C) (U.S. EPA, 2020; Haynes, 2014). The selected value is consistent with the value selected in the *Final Scope of the Risk Evaluation for Dicyclohexyl Phthalate* (1,2-benzenedicarboxylic acid, 1,2-dicyclohexyl ester); CASRN 84-61-7 (also called "final scope for DCHP") (U.S. EPA, 2020).

2.4.2 Auto-Flammability

Data were not identified pertaining to the auto-flammability of DCHP. EPA was not able to select a physical chemistry value for this parameter. No EPI SuiteTM program is available to model auto-flammability. As such, EPA was not able to model or estimate auto-flammability.

2.4.3 Melting Point

EPA extracted and evaluated nine sources containing DCHP melting point information. Four were identified and evaluated as overall high-quality data sources while the remaining five were medium-quality data sources. Three of the high-quality sources reported a value of exactly 66 °C (NLM, 2024b; U.S. EPA, 2019; Haynes, 2014) while the fourth source reported a range of values from 60.2 to 66 °C (Elsevier, 2019). Medium-quality sources reported DCHP melting points from 63 to 67 °C (RSC, 2019a; U.S. EPA, 2019). EPA selected a melting point value of 66 °C as the representative value of the available information obtained from the overall high-quality data sources (Haynes, 2014). The Haynes value of 66 °C was selected since it was an experimental primary data point which was equal to or fell within the range of melting points reported by the other three high-quality sources. The other three high-quality sources existed as either databases or review articles which often re-reported the Haynes value. The selected value is consistent with the value selected in the 2021 final scope for DCHP (U.S. EPA, 2020).

The melting point of DCHP was also modelled using Epi SuiteTM MPBPVP program with a range of output values from 50.36 °C to 116.89 °C and a selected weighted mean melting point value of 64.45 °C (U.S. EPA, 2017). All physical chemistry and fate parameters available for modeling using EPI SuiteTM were modeled given the limited data availability of DCHP physical chemistry and fate values. The modelled estimate reasonably aligns with the final selected experimental melting point of 66 °C. The EPI SuiteTM output is provided in Appendix 4.1.1A.1.

2.4.4 Boiling Point

EPA extracted and evaluated four sources containing DCHP melting point information. Two of the sources were determined to be high-quality sources while the remaining two sources were determined to be medium-quality sources. High-quality sources reported a boiling point of 225 °C (NLM, 2024b; Haynes, 2014). Medium-quality sources reported boiling points ranging from 220 to 476.9 °C (RSC, 2019a, b; EC/HC, 2015). A boiling point value of 225 °C (Haynes, 2014) was selected due to the consensus across the surveyed high-quality sources. The selected value is consistent with the value selected in the final scope for DCHP (U.S. EPA, 2020).

- The boiling point of DCHP was also modeled using Epi SuiteTM MPBPVP program with a value of 395 °C (<u>U.S. EPA, 2017</u>). All physical chemistry and fate parameters available for modelling using EPI SuiteTM were modelled given the limited data availability of DCHP physical chemistry and fate values. The EPI SuiteTM output is provided in Appendix 4.1.1A.1.
 - 2.4.5 Density

EPA extracted and evaluated five sources containing DCHP density information. Two were high-quality sources while the remaining three were medium-quality sources. High-quality sources reported a DCHP density of 1.383 g/m³ (NLM, 2024b; Haynes, 2014). The three medium-quality sources reported DCHP densities ranging from 0.787 to 1.383 g/m³ (RSC, 2019a; EC/HC, 2015). A density value of 1.383 g/m³ was selected because it was the consensus value among the two high-quality sources (Haynes, 2014). The selected value is consistent with the value selected in the final scope for DCHP (U.S. EPA, 2020).

2.4.6 Vapor Pressure

EPA extracted and evaluated six sources containing DCHP vapor pressure information. Five were identified and evaluated as overall high-quality data sources while the remaining source was evaluated as an overall medium-quality data source. The overall high-quality sources reported DCHP vapor pressure values ranging from 9.0×10^{-9} to 5.33×10^{-6} mm Hg (NLM, 2024b; Elsevier, 2019; U.S. EPA, 2019; Gobble et al., 2014; Lu, 2009). The one medium-quality source reported a DCHP vapor pressure value of 0.0998 mm Hg (Cao, 2010). EPA selected a vapor pressure value of 8.69×10^{-7} mm Hg as the representative value of the available information obtained from the overall high-quality data sources (NLM, 2024b, a). The NLM value was selected because it was in range of values from the remaining high-quality sources and the estimated vapor pressure value output from the EPI SuiteTM MPBPVP model (4.58×10^{-6} mm Hg) (U.S. EPA, 2020). The selected value also aligns with the concurrently modeled selected melting and boiling point. The selected value is consistent with the value selected in the final scope for DCHP (U.S. EPA, 2020). The EPI SuiteTM output is provided in Appendix 4.1.1A.1.

2.4.7 Vapor Density

DCHP is a solid at standard temperature (25 °C) and pressure (1 atm). No data were available in the current literature pertaining to the vapor density of DCHP. Since vapor density is not considered a relevant parameter used in the following fate or exposure assessments and Epi SuiteTM does not offer an estimation program capable of estimating vapor density, EPA did not model the vapor density of DCHP.

2.4.8 Water Solubility

EPA extracted and evaluated six sources of water solubility data for DCHP. These sources reported a wide range of solubility values based on modeled and empirical data. Four sources were identified and evaluated as overall high-quality data sources while the remaining two sources were medium-quality data sources.

The overall high-quality sources reported DCHP water solubility values of 1.04 and 4.00 mg/L (NLM, 2024b; U.S. EPA, 2019; EC/HC, 2017; Hollifield, 1979). The reported value of 4.00 mg/L was noted in three of the four sources—one experimental study (Hollifield, 1979) and two databases re-reporting the 4.00 mg/L value from Hollifield (NLM, 2024b; U.S. EPA, 2019; Hollifield, 1979). The value of 1.04 mg/L is reported in Environmental Health Canada (EC/HC, 2017) citing an OECD 105 guideline study for which EPA cannot access the source data.

Two medium-quality sources reported DCHP water solubility values ranging from 0.020 to 4.00 mg/L (EC/HC, 2015; Lu, 2009). One study was a literature review presenting the range of 0.02 to 4.0 mg/L (EC/HC, 2015) while the second source reported a water solubility value of 0.35 mg/L estimated by QSAR (Lu, 2009).

Three of the four high-quality sources (NLM, 2024b; U.S. EPA, 2019; Hollifield, 1979) and one of the three medium-quality sources (EC/HC, 2017) re-report the experimental value reported in (Hollifield, 1979) with a water solubility value of 4.00 mg/L. EPA does not believe that the Hollifield study reasonably reflects the solubility of DCHP because of the use of a chemical dispersant and stabilizer, gum tragacanth, and organic solvent, acetone, in the solution used for DCHP solubility determination (Hollifield, 1979). The use of gum tragacanth in solution, while typically used to prevent micelle formation with oily chemicals, may have altered the water chemistry of the solution and artificially increased the solubility of DCHP by acting as a surfactant (EC/HC, 2015; Hollifield, 1979). Cosolvation such as that demonstrated in Hollifield may allow for the entry of phthalates into surface water and ground water at otherwise achievable concentrations. Other studies have reported a failure to maintain the 4.0 mg/L concentration reported in Hollifield (1979), reporting the solution as unstable with DCHP precipitating out of solution in pure water (KemI, 2023; Mathieu-Denoncourt et al., 2016; EC/HC, 2015). EPA's decision to exclude the Hollifield study based on the uncertainty with the experimental conditions potentially impacting the reported solubility value is supported by multiple studies reporting a solubility lower than that reported in Hollifield (KemI, 2023; Mathieu-Denoncourt et al., 2016; EC/HC, 2015; 1979).

Given the wide range of reported solubility estimates for DCHP, EPA used EPI SuiteTM programs to characterize the range of uncertainty associated with the DCHP solubility based on a variety of physical and chemical parameters. EPI SuiteTM is a standard QSAR tool used by EPA to assess chemicals under TSCA.

Within EPI SuiteTM EPA used two different programs to estimate DCHP water solubility. EPI SuiteTM estimated a range of solubility values from 0.041 to 2.40 mg/L depending on which input parameters were used in the program (*i.e.*, K_{OW}, MP, and MW). WSKOWWIN estimates water solubility using the chemical SMILES and a combination of user-input (EPA-selected) or EPI SuiteTM-estimated melting point, octanol-water partitioning coefficient, and molecular weight (when melting point is not available). WATERNT estimates the water solubility based on the structure (SMILES) fragments. WSKOWWIN is believed to be more reliable than the WATERNT since it accounts for estimated or measured K_{OW}, MP,

and MW values in addition to the chemical structure. The combination of models and input parameters are listed below and summarized in Table 2-2:

- 1. WSKOWWIN estimates water solubility using:
 - a. SMILES code with EPI SuiteTM estimated K_{OW} (6.20) and MW (330.43 g/mol) values,
 - b. SMILES code with EPI SuiteTM estimated K_{OW} (6.20) and EPA selected MP (66 °C),
 - c. SMILES code with EPI SuiteTM EPA selected K_{OW} (4.82) and MW (330.43 g/mol),
 - d. SMILES code with EPA selected K_{OW} (4.82), and melting point (66 °C) values,
- 2. WATERNT estimates water solubility based on a quantitative structure activity relationship.

Table 2-2. EPI Suite™ Model Input/Output Values

Model	Kow	MP (°C)	MW (g/mol)	Solubility (mg/L)
WSKOWWIN	6.20^{a}	N/A ^b	330.43 ^b	0.041
WSKOWWIN	6.20^{a}	66 ^c	N/A	0.0696
WSKOWWIN	4.82^{b}	N/A ^b	330.43 ^b	0.621
WSKOWWIN	4.82^{b}	66 ^c	N/A	1.48
WATERNT	N/A	N/A	N/A	2.40
	WSKOWWIN WSKOWWIN WSKOWWIN	WSKOWWIN 6.20a WSKOWWIN 6.20a WSKOWWIN 4.82b WSKOWWIN 4.82b	ModelKow $(^{\circ}C)$ WSKOWWIN 6.20^a N/A^b WSKOWWIN 6.20^a 66^c WSKOWWIN 4.82^b N/A^b WSKOWWIN 4.82^b 66^c	Model Kow (°C) (g/mol) WSKOWWIN 6.20a N/Ab 330.43b WSKOWWIN 6.20a 66c N/A WSKOWWIN 4.82b N/Ab 330.43b WSKOWWIN 4.82b 66c N/A

SMILES: C1CCC(CC1)OC(=O)c2cccc2C(=O)OC3CCCCC3

A maximum water solubility value of 1.48 mg/L was calculated via EPI Suite'sTM WSKOWWIN estimation program with a known experimentally-determined K_{OW} (4.82) and melting point (66 °C). For phthalates, EPI SuiteTM utilizes data from Howard et al. (1985) to estimate water solubilities based on 14 phthalates of various chain length. In the study, water solubilities estimated from a log K_{OW} between 4 and 6 do not fit along the regression line well and may be less representative of true water solubility. Melting point was not used to estimate water solubility in Howard et al. Howard et al. (1985). However, the WSKOWWIN program was sensitive to both melting point and K_{OW}. Of note, the 1.04 reported by

EC/HC is based on EPI SuiteTM estimate that used an estimated K_{OW} (6.20). A water solubility value of 2.40 mg/L was estimated using the EPI SuiteTM WATERNT estimation program. The EPI SuiteTM

output is provided in Appendix 4.1.1A.2.

Several aquatic toxicity studies note difficulties with keeping DCHP in aqueous solution for the duration of the studies. In one study, the study authors note the true water solubility of DCHP is closer to 30 µg/L (0.03 mg/L) than 1,000 µg/L (1 mg/L) (KemI, 2023; Mathieu-Denoncourt et al., 2016). From the same studies, DCHP was observed to form precipitate at concentrations at or exceeding 30 to 32 µg/L (KemI, 2023; Mathieu-Denoncourt et al., 2016). In addition, ECHA indicates that the maximum realized DCHP water concentrations may be close to 30 µg/L for DCHP (EC/HC, 2017).

Due to the wide range of reported and modeled values and associated uncertainties with study design, EPA selected 0.03 to 1.48 mg/L for the applicable range DCHP solubility in water for use in the draft risk evaluation. The minimum value, 0.03 mg/L, was selected as an observed empirical value reported in the 2016 toxicological study as the perceived lower solubility value with the formation of precipitate observed at concentrations exceeding 0.03 mg/L (KemI, 2023; Mathieu-Denoncourt et al., 2016). While the toxicology study was not explicitly a water solubility study, the source material is considered high in

^a Estimated from Epi Suite™ KOWWIN

^bMW weight used when user-entered MP is not available

^c EPA-selected value

quality by EPA and was the sole study which reported empirical data pertaining to DCHP at lower concentrations ranges. The observed value lower-range value aligns reasonably with the EPI SuiteTM WSKOWWIN value of 0.04 mg/L previously discussed. The 1.48 mg/L value was selected as the upper limit of the selected water solubility range and was selected from the upper range of the EPI SuiteTM SKOWWIN output values (Appendix 4.1.1A.2.2). The value reasonably aligns with the uppermost perceived water solubility value of 1.04 mg/L collected experimentally via OECD 105 as stated by EC/HC (EC/HC, 2017). The EPI SuiteTM value was selected over the EC/HC value because, as a registrant database value, EPA did not have access to the underlying documentation or data related to the reported water solubility value and thus was not able to screen the document for quality assurance measures outside of understanding the standard OECD 105 testing procedures.

Because of the wide range of possible water solubility values, EPA has low confidence in selecting a single value to represent the true solubility of DCHP. But EPA has medium confidence that the EPI SuiteTM WSKOWWIN program-estimated value (1.48 mg/L) represents the upper limit for the solubility of DCHP in water. EPA recognizes this concentration is not likely to occur in the environment but is suitable for screening purposes. The 1.48 mg/L value aligns well with the medium and high-quality sources, including the EH/CH chemical registry (OECD 105 guidelines), which considers the solubility of DCHP in pure water (1.04 mg/L) (EC/HC, 2017). The true solubility of DCHP may be lower than the 1.48 mg/L, with concentrations in the environment expected to be lower based on environmental monitoring data.

2.4.9 Octanol-Water Partitioning Coefficient

EPA extracted and evaluated data from five sources pertaining to the octanol-water partitioning coefficient (K_{OW}) of DCHP. One source was determined to be of high quality with a reported log K_{OW} value of 4.82 (EC/HC, 2017). Three of the sources were determined to be of medium quality with reported log K_{OW} values derived from both experimental data and quantitative structure property relationship models (QSPRs) ranging from 3 to 5.64 (RSC, 2019a; Cao, 2010; Cao, 2010; Cao, 2010). One source was determined to be of low quality with a reported log Cao, value of 5.6 (Cao). A value of 4.82 was selected as the representative log Cao0 value for DCHP with a high overall confidence determination (Cao0 value was selected since it is the sole high-quality experimental value reported in the surveyed literature that reasonably aligns with the values reported in the remaining medium-quality literature values.

The EPI SuiteTM output is provided in Appendix 4.1.1A.3.

2.4.10 Octanol-Air Partitioning Coefficient

EPA extracted and evaluated data from a single source containing information regarding DCHP octanolair partitioning (K_{OA}). The source was determined to be of medium quality with an estimated log K_{OA} value of 9.20 obtained from a QSPR (Lu, 2009). EPA estimated a representative log K_{OA} value of 10.23 using EPI SuiteTM (U.S. EPA, 2017). The EPI SuiteTM estimated log K_{OA} value of 10.23 reasonably aligns with the QSPR-derived estimate of 9.20. As such, EPA has selected the EPI SuiteTM derived value of 10.23 as the representative log K_{OA} value for use in risk assessment (U.S. EPA, 2017). The EPI SuiteTM modeled value was selected because EPI Suite is considered a highly reliable model, with a modeled log K_{OA} value that aligns closely with the reported log K_{OA} value from QSPR modeling. The modeled QSPR value was not selected as it was derived using a limited set of experimental values which did not include DCHP or similar phthalates. The lack of experimental data to confirm either estimated value has led to an overall confidence level determination of medium for the representative log K_{OA} value.

The EPI SuiteTM output is provided in Appendix 4.1.1A.4.

2.4.11 Henry's Law Constant

No data were available in the literature surveyed during systematic review pertaining to the Henry's Law constant for DCHP. EPA estimated a representative Henry's Law constant of 9.446×10⁻⁸ atm·m³/mol at 25 °C via EPI SuiteTM for use as the representative k_h value for DCHP (U.S. EPA, 2017) because no other empirical or modelled values were available. EPI SuiteTM KOHWIN does include a Henry's Law constant of 1.01×10^{-7} atm·m³/mol in the experimental values database (U.S. EPA, 2017); however, the source for the value was not able to be identified for review and no further context was provided by EPI SuiteTM. The database value of 1.01×10^{-7} atm·m³/mol was, as such, not considered a viable experimental value due to the unavailable source and meta data. The EPI SuiteTM output is provided in Appendix 4.1.1A.5.

2.4.12 Air-Water Partitioning Coefficient

EPA extracted and evaluated data from a single source containing information regarding DCHP airwater partitioning (K_{AW}). The source was determined to be of medium quality reporting a log K_{AW} value of –3.56, estimated using a QSPR model (<u>Lu, 2009</u>). Two log K_{AW} values, –4.52 (bond estimate and –5.58 (group estimate), were calculated from the Henry's Law constant, k_h, estimated from the EPI SuiteTM HENRYWIN program (T = 289.15 K, R = 8.205×10⁻⁵ atm-m³/mol-K) (<u>U.S. EPA, 2017</u>). EPA has selected the QSPR-derived value of –3.56 for use as the representative K_{AW} (<u>Lu, 2009</u>). The value was selected with the understanding that no alternative K_{AW} values have been reported in the surveyed literature. The QSPR value has an overall confidence determination of medium due to the lack of phthalate data used to derive the QSPR and the lack of experimental-determined values to support the QSPR value. The QSPR-derived value was selected over the EPI SuiteTM estimated value since EPI SuiteTM currently does not have a program which can directly estimate air-water partitioning values. Instead, the EPI SuiteTM value must be back-calculated indirectly using the Henry's Law Coefficient estimated from Epi Suite'sTM HENRYWINTM program. The EPI SuiteTM output is provided in Appendix 4.1.1A.5.

2.4.13 Octanol-Carbon Partitioning Coefficient

EPA extracted and evaluated data from a single source containing information regarding DCHP octanol-carbon partitioning (K_{OC}). The source was determined to be of medium quality with an estimated log K_{OC} value of 4.47 estimated using a QSPR model (<u>Lu, 2009</u>). Lacking experimental K_{OC} data, the EPA has selected the QSPR-derived value of 4.47 for use as the representative log K_{OC} value. The selected value reasonably aligns with EPI SuiteTM estimates, which range from 3.46 to 4.22 (<u>U.S. EPA, 2017</u>). Lacking adequate experimental data to validate modeled values, EPA has overall medium quality determination in the selected QSPR-derived K_{OC} value. The EPI SuiteTM output is provided in Appendix 4.1.1A.6.

2.4.14 Flashpoint

EPA extracted and evaluated a single source containing DCHP flash point information. The source was determined to be of medium quality with a reported DCHP flash point of 207 °C (RSC, 2019a). Epi SuiteTM does not offer a modelling program with the capacity to estimate chemical flashpoint. As such, flash point was not estimated using Epi SuiteTM. EPA selected a flash point of 207 °C because of the lack of high-quality data (RSC, 2019a). The selected value is consistent with the value selected in the final scope for DCHP (U.S. EPA, 2020).

2.4.15 Viscosity

DCHP is a solid at standard temperature and pressure (25 °C, 1 atm). There were no data in the extracted

literature related to DCHP viscosity and EPA did not determine a viscosity value. Viscosity is not used in the fate or exposure assessments presented.

2.4.16 Refractive Index

EPA extracted and evaluated a single source containing DCHP refractive index information. The source was determined to be of high quality with a reported DCHP refractive index of 1.43 (NLM, 2024b). EPA selected a refractive index of 1.43 for the representative refractive index since it was the only measured value identified in the literature (NLM, 2024b). The selected value is consistent with the value selected in the final scope for DCHP (U.S. EPA, 2020).

2.5 Strengths, Limitations, Assumptions, and Key Sources of Uncertainty for the Physical and Chemical Property Assessment

High quality, experimentally-derived physical and chemical properties were selected whenever possible. When no data were available, peer-reviewed models like EPI SuiteTM and QSPR models were used to estimate the endpoint. These values are not as strong as those experimentally derived, but EPA has high confidence in their EPI SuiteTM derived values because of its robust quality control and extensive training data set used to derive the QSPRs used in the estimation of physical and chemical parameters.

EPI SuiteTM was used to estimate several physical and chemical properties where experimental data were insufficient or contradictory, including: water solubility (Section 2.4.8), log K_{OA} (Section 2.4.12), and Henry's law constant (Section 2.4.11). For water solubility, many of the high and medium quality sources utilized surfactants in their measurement of water solubility, which is believed to have artificially increased the water solubility compared to other standard methods of water solubility measurement. As such, modeled values were included in the assessment and backed with standardized empirical values.

Several values also included the use of QSAR or QSPR. These modeled relationships are frequently informed by chemical data sets with limited representation of phthalates and were assumed to have a lower accuracy compared to empirical data unless otherwise stated.

In all cases, the representative physical and chemical property values were selected based on professional judgement and the overall data quality ranking of the associated references.

3 ENVIRONMENTAL FATE AND TRANSPORT ASSESSMENT OF DCHP

3.1 Approach and Methodology

Reasonably available environmental fate data were reviewed and used in this document to characterize persistence and transport of DCHP in various environmental media. In assessing the environmental fate and transport of DCHP, EPA focused on high and medium quality studies that were identified through systematic review. Information on the full extracted dataset is available in the supplemental file *Draft Risk Evaluation for Dicyclohexyl Phthalate (DCHP) – Systematic Review of Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport (U.S. EPA, 2024a)*.

When data were not available EPA used estimates based on modeling results from EPI SuiteTM (<u>U.S.</u> <u>EPA, 2012</u>), a predictive tool for physical and chemical properties and environmental fate estimation, as noted. EPI SuiteTM input values and modelling information are provided below in Figure 3-1.

Table 3-1. EPI Suite™ Input Values

table 3-1. El 1 Suite input values						
Property	Property Input Value					
Chemical Name	Dicyclohexyl Phthalate	_				
SMILES	C1CCC(CC1)OC(=O)C2=CC=CC=C2C(=O)OC3CCCCC3	_				
Melting Point	66 °C	(<u>Haynes</u> , 2014)				
Vapor Pressure	$8.69 \times 10^{-7} \text{ mmHg}$	(NLM, 2024b)				
Water Solubility	≤1.48 mg/L	(U.S. EPA, 2017)				
Log Kow	4.82	(EC/HC, 2017)				

Several fate parameters were modeled using EPA Epi SuiteTM in addition values collected from the systematic review of existing literature. DCHP fate parameters modeled included hydrolysis first-order degradation rate constant (Section 3.2.1), photolysis first-order degradation rate constant (Section 3.2.2), partitioning to environment (Section 3.3), and atmospheric oxidation rates (Section 3.4.1).

Environmental release and transformation rate constant information is useful for fugacity modeling because the emission rates will predict a real-time percent mass distribution for each environmental medium.

3.2 Transformation Processes

3.2.1 Hydrolysis

Traditionally accepted methods of testing for abiotic hydrolysis of DCHP (OECD Guideline Test 111) are not viable due to the low aqueous solubility of DCHP (ECJRC, 2003a). The low solubility of DCHP led to a lack of viable experimental studies on the hydrolysis of DCHP in ultrapure water or other water matrices. Lacking pertinent data regarding DCHP hydrolysis, the EPI SuiteTM HYDROWIN program was used to estimate the hydrolytic half-life at a pH of 7 and 8 at 25 °C. The EPI SuiteTM HYDROWIN program calculated an estimated hydrolysis half-life of 426 days (1.17 years) at pH 8 and 25 °C, and 4,257 days (11.66 years) at pH 7 and 25 °C (U.S. EPA, 2017). While DCHP hydrolysis was estimated to be greater under caustic conditions, hydrolysis is not expected to be a major route of DCHP transformation under typical environmental conditions. However, higher temperatures, variations from typical environmental pH, and chemical catalysts present in landfill anoxic zones may promote DCHP

- 514 hydrolysis (Huang et al., 2013). Degradation of DCHP in landfills is discussed in Section 3.4.3.3.
- Hydrolysis is not a significant removal mechanism in drinking water (Section 3.5.3) or wastewater
- (Section 3.5.3) treatment processes. Hydrolysis may be a minor removal mechanism in water
- 517 distribution systems following drinking water treatment. In systems with a pH above a value of 8, as
- demonstrated by national surveys of drinking water treatment plants (mean pH = 8.187, max pH = 9.1),
- extended exposure to high-pH waters during distribution could result in minor in-situ degradation of
- 520 DCHP by hydrolysis.

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3.2.2 Photolysis

No experimental values for DCHP photolysis or atmospheric oxidation were identified during the systematic review of existing literature. As such, EPI SuiteTM was used to estimate the atmospheric oxidation half-life of DCHP at 0.441 days (5.288 hours) indicating that atmospheric oxidation may be a significant degradation pathway of DCHP in air. However, DCHP has been observed to undergo some degree of atmospheric transport and has been identified in both indoor and outdoor air. Atmospheric photo-oxidation and transport of DCHP in the atmosphere is discussed more in Section 3.4.1.

Although photolysis may be a route of transformation in the environment, DCHP is not expected to be readily present in the vapor phase in the air due to is high vapor pressure and low Henry's Law constant, thus, limiting photolysis as a major route of transformation in the environment.

3.2.3 Biodegradation and Biotransformation

EPA extracted and evaluated three data sources containing DCHP biodegradation information in water and sediments under aerobic and anaerobic conditions. Two studies evaluating the ready biodegradability of DCHP in water have reported biodegradation ranging from 68.5 to 91 percent in 28 days (t_{1/2}: 8.1–16.8 days) (NCBI, 2020; EC/HC, 2015). One study measured aerobic and anaerobic half-lives for DCHP. Sediment samples were spiked and monitored in a laboratory environment in sealed vials and were extracted using solid media solvent extraction to ensure losses were not due to sorption to sediment (Yuan et al., 2002). The half-lives in sediment under laboratory conditions were reported to be 11.1 and 26.4 days respectively (Yuan et al., 2002). The available information suggests that DCHP will biodegrade faster in aerobic aquatic environments compared with anaerobic aquatic environments, but overall, it is not expected to be persistent in aerobic or anaerobic environment.

Phthalate esters typically degraded to the monoalkyl form under both aerobic and anaerobic conditions (EC/HC, 2015). The monoalkyl product may degrade at a comparable rate to the phthalate ester parent (EC/HC, 2015). Monocyclohexyl phthalate would represent the monoalkyl phthalate that would likely form from the biodegradation of DCHP (U.S. EPA, 2017). No degradation products specific to DCHP were reported in any of the three surveyed sources under aerobic or anaerobic conditions in terrestrial, aquatic, or atmospheric environments.

Table 3-2. Summary of DCHP Biodegradation Studies

Environmental Conditions	Half-Life (days)	Transformation Products	Reference	Overall Data Quality Ranking
Aerobic	8.1 (91% in 28 days, pseudo-first order)	Not Reported	(EC/HC, 2015)	Medium
biodegradation in water	16.8 (68.5% in 28 days, pseudo-first order)	Not Reported	(NCBI, 2020)	Medium

Environmental Conditions	Half-Life (days)	Transformation Products	Reference	Overall Data Quality Ranking
Aerobic biodegradation in saturated sediment	11.1	Not Reported	(Yuan et al., 2002)	High
Anaerobic biodegradation in saturated sediment	26.4	Not Reported	(Yuan et al., 2002)	High

3.3 Partitioning

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3.3.1 Tier I Analysis

Environmental transport and partitioning consist of processes such as volatilization, advection, dispersion, diffusion, association with dissolved organic matter, and sorption to solids. These processes, in turn, are controlled by physical and chemical interactions between DCHP and the surrounding media (*e.g.*, air, water, soil, sediments, etc.). DCHP in the environment is subject to these processes, though some processes are more likely or prevalent than others based on DCHP's physical and chemical characteristics.

To be able to understand and predict the behaviors and effects of DCHP in the environment, the first step is identifying partitioning values (Table 3-3), which can provide insight into how DCHP may favor one media over another. Empirical values were included when available. Estimated values from QSPR models (obtained from literature) and EPI SuiteTM modeling (conducted by EPA) was included when empirical measured data were not available.

Table 3-3. Partitioning Values for DCHP

Parameter	Value ^a	Log Value ^a	Reference	Predominant Phase
Octanol:Water	6.07E4	4.82	(EC/HC, 2017)	Organic Carbon
(Kow)	1.59E6	6.2026 (KOWWIN TM) ^b	(<u>U.S. EPA, 2017</u>)	Organic Carbon
Organic	2.95E4 L/kg	4.47 (QSPR)	(<u>Lu, 2009</u>)	Organic Carbon
Carbon:Water (K _{OC})	1.66E4 L/kg	4.22 (KOCWIN TM) ^b	(<u>U.S. EPA, 2017</u>)	Organic Carbon
Octanol:Air	1.58E9	9.20 (QSPR)	(Lu, 2009)	Organic Carbon
(K_{OA})	1.70E10	10.23 (KOAWIN TM) ^b	(<u>U.S. EPA, 2017</u>)	Organic Carbon
Air:Water (K _{AW})	3.63E-3	-3.56 (QSPR)	(<u>Lu, 2009</u>)	Water

Parameter	Value ^a	Log Value ^a	Reference	Predominant Phase
	3.01E-5	-4.52 (Bond Estimate, HENRYWIN TM) ^b	(<u>U.S. EPA, 2017</u>)	Water
	2.63E-6	-5.58 ^d (Group Estimate, HENRYWIN TM) ^b	(U.S. EPA, 2017)	Water

^a Measured unless otherwise noted.

The value of the partitioning coefficients in Table 3-3 suggest that DCHP will most likely exist primarily sorbed to particulate matter. While the values in Table 3-3 for a specific parameter sometimes span several orders of magnitude, the predominant phase preference of DCHP is consistent across both literature QSPR and EPI SuiteTM estimated values with a clear preference to exist in particulate (organic carbon, sediment, soil, air particulate, dust) over the water and air compartments. Although water does appear to be preferential over air, it is still less favored than the particulate compartments.

DCHP is a solid at environmental temperatures with a melting point of 66 °C (Haynes, 2014) and a vapor pressure of 8.69×10^{-7} mm Hg at 25 °C (NLM, 2024b). DCHP will exist predominantly in the particulate phase with potential to exist in the vapor (gaseous) phase in the atmosphere (EC/HC, 2015). The octanol:air coefficient (K_{OA}) indicates that DCHP will favor the organic carbon present in airborne particles. Based on its physical and chemical properties and short half-life in the atmosphere ($t_{1/2} = 0.44$ days), DCHP was assumed to not be persistent in the air. The AEROWINTM module in EPI SuiteTM estimates that a smaller fraction of DCHP could be sorbed to airborne particulates and these particulates may be resistant to atmospheric oxidation. DCHP may be deposited in surface waters or to the surface of soil through direct deposition of atmospheric particulate resulting in the contamination of soils and surface waters (Zeng et al., 2010). The high estimated K_{AW} value suggests that direct partitioning of gaseous DCHP to precipitation (*i.e.*, atmospheric scavenging) and surface waters is also possible. DCHP fate in indoor and outdoor air and dust will be discussed in further depth in Section 3.4.1.

DCHP may be present in water through release of wastewater treatment plant effluent, through direct deposition from air, or through precipitation (Zeng et al., 2010; Peters et al., 2008). The modest airwater partitioning, and Henry's Law constant suggest that any DCHP present in surface water is unlikely to volatilize to the atmosphere. Any DCHP present in surface water is likely to partition to suspended particulate in water or to sediment particulate with a $K_{\rm OW}$ and $K_{\rm OC}$ higher than 1. In particulate and sediment, DCHP is likely to be shielded from sunlight and unable to undergo abiotic transformation by photolysis but may still be susceptible to transformation through hydrolysis and aerobic and anaerobic transformation. DCHP does have the potential to act like a long-term sink and may de-sorb from sediment if allowed to persist for an extended period such as in biologically inactive dark environments. DCHP fate in sediment, soil, and particulate is discussed in further depth in Sections 3.4.2.2, 3.4.3.1, 3.4.3.2, and 3.4.3.3.

^b Information was estimated using EPI SuiteTM (U.S. EPA, 2017)

^c EPI Suite physical property inputs: MP = 66 °C, BP = 225 °C, VP = 8.69E-7 mm Hg, WS = 1.48 mg/L, Log K_{OW} = 4.82, HLC = 9.446E-8 atm·m³/mole, SMILES:

O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2`

 $[^]d$ Calculated using the relationship HLC = R×T×K_{AW} where R is the universal gas constant equal to 8.206E−5 atm·m³/mol·K

DCHP may be present in soil through the deposition of particulate from the atmosphere (Zeng et al., 2010). Strong sorption also suggests the possibility of DCHP being introduced to soil through the land disposal or application of DCHP-containing biosolids through the treatment of wastewater. Once in soil, DCHP is unlikely to leach with a log K_{OC} value (4.25) greater than 1 suggesting DCHP strongly-sorbs to organic carbon and particulate media. Strong sorption to particulate would also suggest the risk of leaching to groundwater and secondary transport by groundwater is minimal.

3.3.2 Tier II Analysis

TSCA COUs may result in releases of DCHP to air, land, and water. Once released to the environment, the fate and transport characteristics described in prior sections influence in which environmental media compartments DCHP may exist. Based on DCHP's environmental half-lives, partitioning characteristics, and the results of Level III Fugacity modeling using the physical chemistry parameters outlined previously, DCHP is expected to be found predominantly in soil (Table 3-4, Figure 3-1). EPI SuiteTM Tier III Fugacity output is provided in Appendix 4.1.1A.8.

Table 3-4. EPI Suite™ Level III Fugacity Model Output Summary

Release Scenario	Release Rate (kg/hr)	Air (Percent)	Water (Percent)	Soil (Percent)	Sediment (Percent)
Equal Release	1000	0.2	13.2	76.4	10.2
100% Air Release	1000	1.4	2.4	94.3	1.85
100% Soil Release	1000	< 0.01	0.05	99.9	0.04
100% Water Release	1000	< 0.01	56.5	0.04	43.5

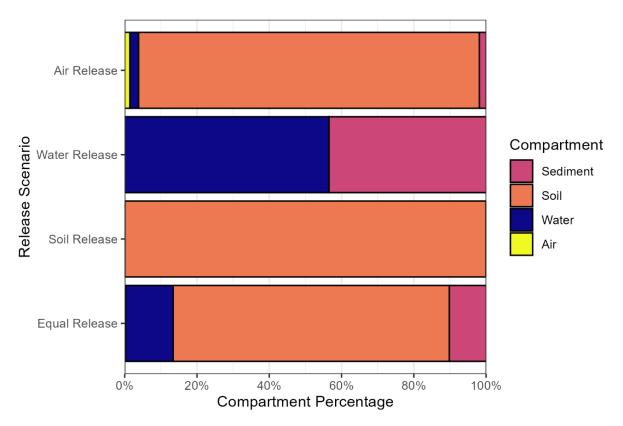


Figure 3-1. EPI Suite TM Level III Fugacity Model Graphical Summary

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DCHP may be released to the atmosphere through stack or fugitive air emissions. Once in the atmosphere, DCHP is likely to partition to particulate matter suspended in the atmosphere, partition to water and soil directly, or may be scavenged by precipitation. The fraction of DCHP which remains in the atmosphere is likely to undergo indirect photolysis or hydrolysis to form monocyclohexyl phthalate and cyclohexanol via acid-ester hydrolysis and indirect photolysis.

DCHP may reach surface waters through deposition of atmospheric DCHP or by release of wastewater effluent and has been observed in surface waters both in the United States and internationally. DCHP is not likely to be persistent in surface water may be biologically degraded aerobically or anaerobically in tandem with abiotic processes to form monocyclohexyl phtalate and cyclohexanol. DCHP is also likely to partition to suspended and benthic sediments from surface water which may act as a long-term sink. DCHP is unlikely to volatilize from water or partition to soil.

DCHP is expected to exist in sediments primarily through sorption from waters containing DCHP. It is unlikely that DCHP will transform abiotically via photolysis but may degrade via hydrolysis to form monocyclohexyl phthalate and cyclohexanol. Like in surface waters, DCHP has been shown to degrade biologically under both aerobic and anaerobic conditions as well as abiotically.

DCHP is not expected to be present in groundwater and thus far has not been observed in groundwater in the United States or abroad. DCHP could be introduced to groundwater by infiltration of precipitation or surface waters. In groundwater, DCHP would likely partition largely to the particulate and organic fraction of soil with limited de-sorption, highly retarding its transport and keeping it locally contained. As in sediments, DCHP may degrade biologically under aerobic or anaerobic conditions as well as by hydrolysis and is not expected to be persistent.

DCHP may be introduced to soil by deposition from the atmosphere or through precipitation. It may also be directly incorporated into the soil through the land application of biosolids. DCHP is expected to largely remain within soil with little-to-no de-sorption or leaching. DCHP can be degraded biologically or by hydrolysis. Photolysis will impact DCHP sorbed in the uppermost layer of soil exposed to the sun but would otherwise not impact deeper layers. DCHP is not expected to volatilize to the atmosphere from soil or pore water.

DCHP may be introduced to landfills through consumer waste, industrial waste, dewatered wastewater sludge, stabilized biosolids, or incinerated sludge. DCHP is not expected to leach significantly and will likely sorb to the particulate and organic matter present in the landfills and surrounding liners. DCHP is likely to degrade biologically and through photolysis in upper parts of the landfills, but lower sections of the landfills may not be suitable for biologic degradation. In lower landfills, hydrolysis will likely be the sole method of degradation and may result in high persistence.

 In wastewater, DCHP has been observed to be removed primarily through sorption to organic material and removal via sludge. Some minor removal may be attributed to biologic degradation or abiotic processes; however, the limited hydraulic retention time would result in limited mass reduction. DCHP has been observed in wastewater effluent which may pass DCHP into surface water. DCHP may also be present in the sludge line where it may be placed in a landfill or on land applied as biosolids. Volatilization of DCHP through turbulent flow or aeration of wastewater is unlikely and is not

Each of the pathways will be discussed in further detail in the remainder of the present analysis.

considered a significant transport pathway.

3.4.1 Air and Atmosphere

As described in the Draft Environmental Release and Occupational Exposure Assessment for Dicyclohexyl Phthalate (DCHP) (U.S. EPA, 2024c), DCHP may be released to air from TSCA COUs. When released to air, DCHP is not expected to persist in the gaseous form. Instead, DCHP may sorb to particulates or solidify, settling out of the air. DCHP may be present in particulate suspended in air (EC/HC, 2017). DCHP is susceptible to photo-oxidation, but the half-life is not fast enough to limit exposure near releasing facilities and photolysis is expected to be limited in indoor environments. Photooxidation occurs on the surface of air particulate. While photo-oxidation of DCHP in the gas phase is possible, DCHP is not expected to be readily present in the gas phase due to the low Henry's law constant and small octanol-air partitioning coefficient. Photo-oxidization may also be limited because of competing sorption processes. The EPI SuiteTM AEROWINTM model predicts that 25.1 percent to 44.9 percent of atmospheric DCHP may be sorbed to particulate material (U.S. EPA, 2017). Any DCHP sorbed to particulates in air is not expected to be susceptible to photo-oxidation as it may be shielded from direct sunlight. While it may degrade rapidly due to photo-oxidation, some medium-to-long transport of DCHP is still possible. DCHP in the atmosphere may be deposited into surface water bodies or soil with a measured flux of 0.088 to 0.433 μ g/m²-day (Zeng et al., 2010). Precipitation (e.g., rain) may also scavenge DCHP from the atmosphere and deposit it into surface water or soils (Peters et al., 2008).

In general, phthalate esters are ubiquitous in the atmosphere and indoor air. Their worldwide presence in air has been documented in the gas phase, suspended particles, and dust (Net et al., 2015). Most of the studies reported DCHP to be the predominant phthalate ester in the environment. It is likely that DCHP behaves like other phthalates in indoor air and dust due to its similar partitioning coefficients and volatility. Studies on other phthalates suggest that indoor air and dust are likely to have higher concentrations of phthalates compared to their outdoor counterparts in part due to the potential releases of phthalates indoors (Kubwabo et al., 2013; Wang et al., 2013; Abb et al., 2009). Concentrations of DCHP in indoor and outdoor air and dust are likely to follow similar trends with higher concentrations in occupied homes with large quantities of plastics, homes that have recently undergone construction or in non-residential indoor sites (e.g., restaurants, schools, hospitals, commercial stores) using DCHP-containing products. The fate and transport of DCHP in indoor (Section 3.4.1.1) and outdoor air (Section 3.4.1.2) and dust will be discussed in further detail in the subsequent sections.

3.4.1.1 Indoor Air and Dust

There are several studies examining the concentration of DCHP in indoor air particulate and dust. Only two studies were conducted within the United States. The US studies are summarized below, and the international monitoring studies are provided in Appendix 4.1.1B.1. The foreign studies are not discussed further since it is unclear how environmental factors contributing to DCHP media concentrations may vary between the United States and other countries. However, the international studies do support that DCHP is detected in indoor air and dust.

Two U.S. studies examined indoor dust for the presence of DCHP. One 2001 survey of six offices in the United States identified DCHP in all six locations with a mean DCHP concentration in dust suspended in air of 1.86 ± 1.62 mg/kg (0.569-5.38 mg/kg) (Rudel et al., 2001). In another survey collecting settled dust that had been swept or vacuumed for analysis, DCHP was identified in 18 percent of U.S. samples (n = 33 indoor sites) below 0.3 mg/kg dw (Guo and Kannan, 2011). The same study reported measured concentrations of DCHP in dust from 75 indoor sites in China, also reporting concentrations below 0.3

mg/kg dw. There was no statistical difference in the detection frequency nor concentration of both DCHP and total phthalates between the United States and China (Guo and Kannan, 2011).

3.4.1.2 Outdoor Air and Dust

There are several studies examining the concentration of DCHP in outdoor air and dust; however, none of the studies collected during systematic review originated from the United States. Five international studies identified DCHP in outdoor air particulate and dust samples in surveys located in China (2 studies), Turkey (1 study), South Korea (1 study), and Spain (1 study). The specific concentration values from these studies were not taken into consideration in the present analysis since it is unclear how environmental factors contributing to DCHP media concentrations may vary between the United States and other countries. These studies do support that DCHP may be found in air particulate and dust in outdoor environments. Key findings of the five international studies are provided in Appendix B.2.

3.4.2 Aquatic Environments

3.4.2.1 Surface Water

As described in the *Draft Environmental Release and Occupational Exposure Assessment for Dicyclohexyl Phthalate (DCHP)*, DCHP may be released to surface water from TSCA COUs but is generally released in low quantities (<u>U.S. EPA, 2024c</u>). It is possible for DCHP to reach surface water through atmospheric deposition, precipitation, and through wastewater treatment plant discharge (<u>Wu et al., 2019</u>; <u>Peters et al., 2008</u>). If DCHP enters surface water, it is expected to partition to suspended organic material present in the water column and sediment (Section 3.3). High concentrations of DCHP have been found in the particulate and biosolids in wastewater treatment while biodegradation of DCHP in activated sludge was observed to have a significantly smaller impact on the reduction of DCHP concentrations in water.

There is very limited monitoring data for DCHP in surface waters reported to monitoring databases such as the Water Quality Portal which did not include measured concentrations of DCHP in surface water. DCHP was queried using all known names and CAS numbers related to DCHP with no results. In addition, a 2021 survey of phthalates in Washington state water bodies did not measure concentrations of DCHP in water above reporting limits (0.51 ug/L) (WA DOE, 2022). One reference measured DCHP in dissolved water concentrations in surface waters in the United States and Canada. Seawater samples with column concentrations of up to 15 ng/L DCHP were measured in Puget Sound, WA and Barkley Sound, BC (Keil et al., 2011). Several international studies from China (3), South Korea (1), Kuwait (1), and The Netherlands (1) also identified DCHP in surface water bodies. While the international studies do support the idea that DCHP may be present in surface water and suspended particulate, the specific values may not be a viable direct comparison to the United States. As such, details of the international studies extracted during systematic review are not included in this section but are reported in further detail in Appendix B.3.

DCHP is susceptible to hydrolysis (Section 3.2.1) to form monocyclohexyl phthalate and cyclohexanol via avid ester hydrolysis with an estimated half-life of 426 days at pH of 7. However, the hydrolytic half-life of DCHP would mean hydrolysis is not a major pathway for degradation in all circumstances except for water bodies with no light penetration and no biotic activity. No data was identified related to direct photolysis of DCHP. While atmospheric oxidation (indirect photolysis) was estimated using EPI SuiteTM (Section 3.2.2), it is unclear if the estimated atmospheric transformation degradation rate would translate to aquatic environments. It is likely that photolysis may result in the abiotic transformation of DCHP to monocyclohexyl phthalate and cyclohexanol in shallow waters with adequate light penetration. Photolysis would not be a viable abiotic transformation pathway for deeper waters with limited or no

light penetration. DCHP is susceptible to biotic degradation in both the water column and in sediment but may persist for days to weeks. However, binding to sediment reduces the bioavailability of DCHP in soils and sediments which may increase the persistence.

3.4.2.2 Sediments

DCHP may exist in sediments following releases to surface waters as described in the release assessments (<u>U.S. EPA, 2024c</u>). Once in water, the EPI SuiteTM level III fugacity model suggests that up to 43.5 percent of total DCHP mass may sorb to sediments (Section 3.3.2). There is no known TRI data which suggests that DCHP would be directly released to sediments.

No peer-reviewed monitoring studies were identified in systematic review measuring the concentration of DCHP in sediment samples within the United States. Several international studies have measured DCHP in sediment and pore water concentrations. While the studies do support the presence of DCHP in sediments with concentrations typically comparable or significantly higher that of the surrounding water, the specific measured values would be unlikely to be a viable direct comparison to the United States. As such, the specific measured values were not included in the present analysis but may be found in Appendix B.4. While literature values were limited, the Water Quality Portal was queried for data pertaining to DCHP in sediments. In the WQP, the State of Washington reported DCHP monitoring data in sediment for 33 sediment samples from April 5th to June 15th of 2021. Two samples reported DCHP above the reporting limit (RL) with concentrations of 66.5 and 73.7 μ g/kg. Reporting limits for the Washington state monitoring program varied widely, ranging from 30.1 to 93 μ g/kg.

Based on the water solubility (\leq 1.48 mg/L) and affinity for sorption to organic matter (log K_{OC} = 4.12), DCHP will partition to the organic matter present in soils and sediment when released into the environment but to a lower extent than other more hydrophobic phthalate esters such as DEHP. The available information suggests that DCHP could remain longer in subsurface sediments compared with water. In terrestrial and aquatic environments, DCHP is not expected to be persistent, unless located proximal to areas of continuous release, such as a surface water body receiving discharge from a municipal wastewater treatment plant. In addition, DCHP sorbed to suspended or benthic sediments may be less bioavailable for degradation and hence persist longer in the environment (Kickham et al., 2012). Due to the hydrophobicity of DCHP (Log K_{OW} = 4.82) and its physical form at environmentally relevant temperatures (solid), it is expected to be found predominantly in sediments near point sources, with a decreasing trend in sediment concentrations downstream. Similarly, significant quantities of DCHP sorbed to sediment may act as a long-term reservoir and source to contaminated water bodies.

Once in sediments, DCHP degrades under both aerobic and anaerobic conditions with one study reporting sediment half-lives of 11.1 days in aerobic conditions and 26.4 days under anaerobic conditions. While transformation products were not provided, EPA Chemical Transformation Simulator predicts that the monoalkyl variant, monocyclohexyl phthalate, would be the primary biological transformation product long with cyclohexanol (U.S. EPA, 2017). More detail on the biodegradation of DCHP is provided in Section 3.2.3. DCHP may degrade to form monocyclohexyl phthalate and cyclohexanol via acid ester hydrolysis. With a half-life of 426 days at a pH of 7, hydrolysis would likely be a minor pathway in and sediments and pore-spaces with any significant biotic activity.

3.4.3 Terrestrial Environments

3.4.3.1 Soil

DCHP may be present in soil through various means. DCHP has been observed to deposit directly from the atmosphere to soil (Zeng et al., 2010; Vethaak et al., 2005). Although no TRI data has reported the

field application of biosolids, DCHP has been shown to exist in wastewater sludge and final biosolids and may be incorporated directly into soil following biosolids land applications (Wu et al., 2019; Zhu et al., 2019; Meng et al., 2014). The EPI SuiteTM level III fugacity model estimates that DCHP released directly to soil will overwhelmingly remain in the soil with a calculated 99.9 percent of applied DCHP remaining in soil (Section 3.3.2). DCHP may also partition to soil when released to other environmental compartments; EPI SuiteTM estimated 76.4 of DCHP released to air may be deposited in soil. Releases to water, however, are believed to partition largely to sediment with less than 1 percent of DCHP partitioning to soil. As such, DCHP is expected to be deposited to soil via two primary routes: application of biosolids and sewage sludge in agricultural applications or sludge drying applications, and atmospheric deposition. DCHP has a Henry's law constant of 9.446×10⁻⁸ atm·m³/mol at 25 °C and is not likely to volatilize from soils once incorporated.

DCHP shows an affinity for sorption to soil and its organic constituents (log K_{OC} of 4.47, log K_{OW} of 4.82). Given that these properties indicate the likelihood of sorption to organic carbon present in soil, DCHP is expected to have low mobility in soil environments.

No studies were identified surveying the presence of degradation of DCHP in soils within the United States. Five studies reported the presence of DCHP in China. While these studies demonstrate that DCHP may be present in soil, it is unlikely that the international studies are appropriate for a direct comparison to the United States release scenarios and were subsequently not included in the present analysis. The details of the studies were reported in Appendix B.5.

No studies were found with measured half-life values for DCHP in soil however the half-life of DCHP in soil is expected to be similar if not shorter than the measured half-life in sediments (11.1–26.6 days, Section 3.2.3). Thus, DCHP is not expected to persist in soils but as with sediments, DCHP sorbed to soil has the potential to persist longer in the environment than free DCHP in surface water, groundwater, or air.

3.4.3.2 Biosolids

Sludge is defined as the solid, semi-solid, or liquid residue generated by wastewater treatment processes. The term "biosolids" refers to treated sludge that meets the EPA pollutant and pathogen requirements for land application and surface disposal and can be beneficially recycled (40 CFR Part 503) (U.S. EPA, 1993). DCHP is expected to sorb largely to biosolids during wastewater treatment because of its potential for sorption to particulate and organic media (log $K_{OW} = 4.82$; log $K_{OC} = 4.47$) and low water solubility (\leq 1.48 mg/L). DCHP, like other phthalates, is expected to partition to biosolids in wastewater treatment and subsequently be removed by physical separation processes (*e.g.*, sedimentation, filtration, dewatering, sludge thickening). The resulting biosolids would likely have an appreciable fraction of the initial DCHP in the influent.

Current reporting data indicates that biosolids are likely to be removed, either incinerated or dried, and transferred to landfill. There are no reported TRI data indicating that phthalate containing biosolids have been applied to land in agricultural settings or otherwise removed by land disposal. Landfill disposal of biosolids will be discussed in Section 3.4.3.3. No U.S. studies have identified DCHP in wastewater activated sludge or biosolids. Several international studies in China have identified DCHP in biosolids and sludge. The studies do support the capacity of biosolids to store and remove DCHP from water in wastewater treatment and its presence in final biosolids, however the data may not accurately reflect the concentrations of DCHP in American wastewater treatment systems and thus have not been included in the present analysis. Details for the international studies are provided in Appendices B.6 and B.9.

If applied to land as biosolids, DCHP is expected to have low mobility due to its high tendency to sorb to organic matter and particulate, and due to its limited water solubility. Similarly, DCHP is not expected to be readily bioavailable when it is incorporated into soil via biosolids. Once incorporated, DCHP does appear to have potential for biodegradation under aerobic conditions, such that would exist in shallow soils, with a reported half-life of 8.1 to 16.8 days in aerobic, moist soils (NCBI, 2020; EC/HC, 2015). Biodegradation is expected to be more persistent in anaerobic soils, with a half-life of 26.4 days in anaerobic soils (Yuan et al., 2002). There is limited information available related to the uptake and bioavailability of DCHP in land applied soils. DCHP's solubility and sorption coefficients suggest that bioaccumulation and biomagnification will not be of significant concern for exposed organisms. Bioaccumulation and biomagnification will be discussed further in Section 3.6.

3.4.3.3 Landfills

 For the purpose of this assessment, landfills will be considered to be divided into two zones: an "upper-landfill" zone with normal environmental temperatures and pressures, where biotic processes are the predominant route of degradation for DCHP; and a "lower-landfill" zone where elevated temperatures and pressures exist and abiotic degradation is the predominant route of degradation. In the upper-landfill zone where oxygen might still be present in the subsurface, conditions may still be favorable for aerobic biodegradation; however, photolysis and hydrolysis are not considered to be significant sources of degradation in this zone. In the lower-landfill zone, conditions are assumed to be anoxic, and temperatures present in this zone are likely to inhibit anaerobic biodegradation of DCHP. Temperatures in lower landfills may be as high as 70 °C—at temperatures at and above 60 °C, biotic processes are significantly inhibited and are likely to be completely irrelevant at 70 °C (Huang et al., 2013).

DCHP is deposited into landfills from consumer products containing DCHP and as biosolids containing DCHP from wastewater treatment. DCHP's expected maximum water solubility of 1.48 mg/L suggests it might be present in small concentrations in landfill leachate. Hydrolysis will likely not be a major degradation pathway for degradation of DCHP in leachate with an estimated hydrolysis half-life of 11.66 years at a pH of 7 and at 25 °C (U.S. EPA, 2017). Hydrolysis might play a more significant role in the lower landfill with increased temperatures increasing the rate of DCHP degradation to monocyclohexyl phthalate and cyclohexanol via carboxylic acid ester hydrolysis (U.S. EPA, 2017).

DCHP may degrade biologically via aerobic degradation in the upper landfill where aerobic conditions dominate. Although literature is limited, some studies suggest DCHP is capable of being aerobically degraded with an aerobic half-life ranging from 8.1 to 16.8 days in oxygen rich, moist soils (NCBI, 2020; EC/HC, 2015). DCHP may degrade at a slower rate in the anoxic lower landfill with a reported half-life of 26.4 days in anaerobic, moist soils (Yuan et al., 2002). However, as previously noted above, biological degradation would be limited by high temperatures exceeding the habitable zone of bacteria (Huang et al., 2013). In the case of high-temperature biodegradation (<60 °C), DCHP would likely be persistent with slow hydrolytic degradation and no biological degradation.

3.4.3.4 Groundwater

Potential sources for DCHP in groundwater include wastewater effluent, landfill leachate, deep well disposal, or infiltration from surface water. Diffuse sources include stormwater runoff and runoff from biosolids applied to agricultural land.

No studies have been identified measuring DCHP in groundwater. However, data has been reported on the presence of DCHP in possible groundwater sources, including wastewater effluent, surface water, precipitation, and in sediments (Sections 3.4.2.1, 3.4.2.2, 3.4.3.4, and 3.5.3, respectively).

DCHP's high potential to sorb to soil and sediment particulate and organic media ($\log K_{\rm OW} = 4.82$; $\log K_{\rm OC} = 4.47$) will significantly limit DCHP's mobility, resulting in subsequently high retardation in groundwater (EC/HC, 2017; Lu, 2009). Transport in groundwater is further limited by DCHP's water solubility and solid physical state which may cause precipitation leading to void blockage in regions with high concentrations of DCHP and dissolved minerals (*i.e.*, high ionic strength) (U.S. EPA, 2017; Haynes, 2014). Significant long-distance transport is unlikely due to the solid state of DCHP in environmental conditions.

DCHP may be present at larger concentrations if it is introduced along with organic solvents or alcohols in a plume containing multiple contaminants. In the event of co-solvation, DCHP may be present at higher concentrations in groundwater and more susceptible to groundwater conveyance. However, no studies or data were identified indicating such a presence of DCHP in groundwater contaminant plumes resulting from the co-solvation of DCHP with organic solvents or alcohols.

It is likely that DCHP will be moderately persistent in groundwater where it is present in appreciable concentrations. DCHP has a reported anaerobic half-life ranging from 11.1 to 26.4 days in aerobic and anaerobic saturated sediments with a comparable half-life anticipated in groundwater (NCBI, 2020). DCHP can also degrade to some extent via carboxylic acid ester hydrolysis to form monocyclohexyl phthalate and cyclohexanol (https://qed.epa.gov/cts/), however the rate of such degradation is unknown.

3.5 Persistence Potential

DCHP is not expected to be persistent in the environment as it is expected to degrade rapidly under most environmental conditions with delayed biodegradation in low-oxygen media. In the atmosphere, DCHP is unlikely to remain for long periods of time as it is expected to undergo photolytic degradation through reaction with atmospheric hydroxyl radicals, with estimated half-lives of 5.28 hours. DCHP is predicted to hydrolyze slowly at ambient temperature and environmentally relevant pH levels but is not expected to persist in aquatic media as it undergoes rapid aerobic biodegradation (Section 3.4.2.1). DCHP has the potential to persist for longer periods of time in soil and sediments, but due to the inherent hydrophobicity (log $K_{OW} = 4.82$) and sorption potential (log $K_{OC} = 4.47$), it is not expected to be bioavailable for uptake. Using the Level III Fugacity model in EPI SuiteTM (LEV3Epi) (Appendix A.10), DCHP's overall environmental half-life was estimated to be approximately 64 days (U.S. EPA, 2017). Therefore, although DCHP is not expected to be persistent in the atmosphere or in surface, it might persist in sediments or soil.

3.5.1 Destruction and Removal Efficiency

Destruction and Removal Efficiency (DRE) is a percentage that represents the mass of a pollutant removed or destroyed in a thermal incinerator relative to the mass that entered the system. EPA requires that hazardous waste incineration systems destroy and remove at least 99.99 percent of each harmful chemical in the waste, including treated hazardous waste (46 FR 7684) (Federal Register, 1981).

Currently there is no information available on the DRE of DCHP. However, the DCHP annual releases from a Danish waste incineration facility were estimated to be 9 percent to air and 91 percent to municipal landfill (ECJRC, 2008). These results suggest that DCHP present during incineration processes will very likely be released to landfills with a small fraction released to air. Based on inherent hydrophobicity and high sorption potential, DCHP released to landfills is expected to partition into the landfills' organic matter. Similarly, DCHP released to air is expected to partition to soil and sediments as described in Sections 3.4.2.2 and 3.4.3.1, as well as rapidly react via indirect photochemical processes within hours (U.S. EPA, 2017). In addition, DCHP adsorbed to sediments and soils is not expected to be

bioavailable for uptake, and the fraction that does not adsorb will biodegrade easily (<u>Kickham et al.,</u> 2012).

3.5.2 Removal in Wastewater Treatment

Wastewater treatment is performed to remove contaminants from wastewater using physical, biological, and chemical processes. Generally, municipal wastewater treatment facilities apply primary and secondary treatments. During the primary treatment, screens, grit chambers, and settling tanks are used to remove solids from wastewater. After undergoing primary treatment, the wastewater undergoes a secondary treatment. Secondary treatment processes can remove up to 90 percent of the organic matter in wastewater using biological treatment processes such as trickling filters or activated sludge. Sometimes an additional stage of treatment such as tertiary treatment is utilized to further clean water for additional protection using advanced treatment techniques (*e.g.*, ozonation, chlorination, disinfection).

STPWINTM, an EPI SuiteTM module that estimates chemical removal in sewage treatment plants was used to estimate DCHP removal during wastewater treatment. An estimated DCHP removal efficiency of 71.2 percent in conventional wastewater treatment processes biodegradation of DCHP in activated sludge accounting for 0.63 percent of the 71.2 percent overall removal. Sludge absorption accounts for the remaining 70.6 percent of DCHP removal. The model aligns well with the substantial sorption that would be predicted from the high sorption to particulate and organic carbon (log $K_{ow} = 4.82$; log $K_{oc} = 4.47$) and low water solubility (≤ 1.48 mg/L).

Overall, DCHP is primarily removed from wastewater via the accumulation and removal of biosolids and sludge with limited removal from biodegradation. Membrane-based biological treatment systems appear to have higher removal compared to conventional biological treatment due to the filtration by the membrane, but not enough information is currently available to make a final degermation in specific technology removal efficiency. DCHP will likely be present in any biosolids generated from wastewater treatment. TRI data is not available for DCHP related to biosolids disposal. However, common disposal methods for wastewater biosolids containing other phthalates include landfill disposal and deep well injection. Land application or incineration have not been reported for any phthalate containing biosolids but are viable alternative disposal methods for municipal biosolids. DCHP in biosolids is discussed in Section 3.4.3.2 while landfills are discussed in Section 3.4.3.3.

EPI SuiteTM output for STPWIN is provided in Appendix A.10.

3.5.3 Removal in Drinking Water Treatment

Drinking water in the United States typically comes from surface water (*i.e.*, lakes, rivers, and reservoirs) and groundwater. The source water then flows to a treatment plant where it undergoes a series of water treatment steps before being dispersed to homes and communities. In the United States, public water systems often use conventional treatment processes that include coagulation, flocculation, sedimentation, filtration, and disinfection, as required by law.

Very limited information is available on the removal of DCHP in drinking water treatment plants. No data was identified by the EPA for DCHP in drinking water. Based on the water solubility ($\leq 1.48 \text{ mg/L}$) and high log K_{OW} (4.82), DCHP in water is expected to partition to suspended solids present in water. This is supported by the Level III Fugacity model in EPI SuiteTM (Appendix A.8), which predicts that 43 percent of DCHP released to water will partition to sediments (U.S. EPA, 2017). This data suggests that conventional drinking water treatment systems may not be efficient at removing DCHP from drinking water although prolonged retention of drinking water in storage tanks in the presence of free available

residual chlorine has been shown to be beneficial in reducing the concentrations of phthalates in the water (Kong et al., 2017; Yang et al., 2014).

According to the EPA Drinking Water Treatability Database (https://www.epa.gov/water-research/drinking-water-treatability-database-tdb), membrane separation, activated carbon and advanced oxidation are potential treatment options with varying degrees of effectiveness for DCHP.

3.6 Bioaccumulation Potential

Based on the low water solubility (\leq 1.48 mg/L) and high hydrophobicity (log K_{OW} = 4.82; log K_{OC} = 4.47), DCHP is expected to have low bioaccumulation potential, low biomagnification potential, and low potential for uptake. This was supported by results from the BCFBAF module in EPI SuiteTM, which predicts a log BCF of 2.85 and log BAF of 1.83 for DCHP ($\underline{\text{U.S. EPA, 2017}}$).

The EPA found no data sources reporting the aquatic bioconcentration, aquatic bioaccumulation, aquatic food web magnification, terrestrial biota-sediment accumulation, and terrestrial bioconcentration of DCHP. One source reported DCHP concentrations of 0.11 ug/g wet-weight in green sunfish tissue found in a recreational fishery in metro-Phoenix. Twenty-one fishes were sampled from 11 fisheries within metro-Phoenix. Although phthalates were found in all of the sampled fishes, only the green sunfish from one of the fisheries was found to have measured concentrations of DCHP. Green sunfish was noted to be a resident fish, which means it was introduced but not annually re-stocked such that the measured concentrations can be safely assumed to be due to exposure within the recreational fishery. That might partly explain why of all of the sampled fish, green sunfish was the fish species with the highest number as well as the highest concentrations of different phthalates (Lucas and Polidoro, 2019). The presence of DCHP in green sunfish does suggest that it is bioavailable in aquatic environments; however, the estimated BCF/BAF suggests that DCHP does not meet the criteria to be considered bioaccumulative (BCF/BAF > 1,000). Bioaccumulation and bioconcentration in aquatic and terrestrial organisms are not expected to be important environmental processes for DCHP. This conclusion is consistent with the observations made for other phthalates with measured BCF/BAFs.

EPI SuiteTM output for STPWIN is provided in Appendix A.10.

3.7 Overall Fate and Transport

The inherent physical and chemical properties of DCHP govern its environmental fate and transport. Based on its aqueous solubility, slight tendency to volatilize, and strong tendency to adsorb to organic carbon, DCHP will preferentially sorb to sediments, soils, particulate matter in air, and wastewater solids during wastewater treatment. Soil, sediment, and sludge/biosolids are predicted to be the major receiving compartments for DCHP as indicated by physical and chemical and fate properties, partitioning analyses, and as verified by monitoring studies.

If released into the atmosphere, DCHP is expected to partition to particulate in the air or be deposited into adjacent water bodies and soil. DCHP may degrade somewhat by photolysis; however, photolysis is expected to be hindered for any DCHP absorbed to particulate media which is shielded from sunlight. DCHP is expected to be present in higher concentrations in indoor air and dust, where it is protected from sunlight and biodegradation, with concentrations elevated by the indoor use of DCHP, and limited long-distance conveyance compared to outdoor air.

Aqueous transportation of DCHP in surface water, as landfill leachate, in drinking water influent, and in wastewater effluent may all be minor pathways for short-range transport. However, DCHP in water is

expected to partition out of the water phase and adsorb to particulate and organic material, including benthic sediments, soils, and suspended solids, leading to immobilization of DCHP and hindering long-range transport. In areas where continuous releases of phthalates occur such as in the streams receiving wastewater treatment plant effluent, higher levels of phthalates in surface water can be expected, trending downward distally from the point of releases with parallel concentration trends in the receiving body sediments.

DCHP is expected to be removed from wastewater during wastewater treatment largely by adsorption and absorption to biosolids and particulate media, via physical means such as sedimentation or clarification, or by membrane filtration. Biological degradation is expected to be a minor pathway for DCHP in wastewater treatment due to the long aerobic and anaerobic half-lives of DCHP relative to a typical wastewater treatment hydraulic half-life and mean cellular residence times. Off-gassing is unlikely to be a significant removal mechanism due to DCHP's low volatility and low Henry's Law constant.

Biodegradation would be further hindered in anoxic or anaerobic conditions, such as would be found in benthic sediments, groundwater, and in lower landfills. Anaerobic conditions would increase the persistence of DCHP, with the primary method of degradation limited to hydrolysis.

4 WEIGHT OF SCIENTIFIC EVIDENCE CONCLUSIONS FOR FATE AND TRANSPORT

4.1.1 Strengths, Limitations, Assumptions, and Key Sources of Uncertainty for the Fate and Transport Assessment

High-quality measured and experimentally derived fate properties were selected whenever possible. When no data were available, peer-reviewed models such as EPI SuiteTM and QSPR models were used to estimate the parameter values. These values are not as strong as those experimentally derived, but EPA has high confidence in their selection. High-quality field data was used to support the findings of the analyses wherever possible.

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Given the consistent results from numerous high-quality studies, there is a robust confidence that DCHP

- may degrade to monocyclohexyl phthalate and cyclohexanol (Sections 3.2.1, 3.2.2, and 3.2.3), and
- will not significantly degrade via hydrolysis (Section 3.2.1) under standard environmental conditions,
- may degrade by photolysis (Section 3.2.2) in environments with significant sunlight exposure,
- will readily degrade in anaerobic or anoxic conditions (Section 3.2.3), and
- may be susceptible to long-range transport and deposition to water and soil via the atmosphere (Section 3.4.1),
- will partition to organic particulate in indoor and outdoor air (Sections 3.4.1.1 and 3.4.1.2), and
- will partition to organic particulate with limited mobility in sediment (Section 3.4.2.2), soil (Section 3.4.3.1), biosolids (Section 3.4.3.2), landfills (Section 3.4.3.3), and groundwater (Section 3.4.3.4).

As a result of limited studies identified, there is a moderate confidence that DCHP

- will be readily removed in wastewater treatment with a small fraction passing through to the effluent and a large portion being sorbed to biosolids (Sections 3.4.3.2 and 3.4.3.3), and,
- may be removed through drinking water treatment by sorption to organics and particulate filtration and membrane separation (Sections 3.5.2 and 3.5.3), and
- is likely to be bioaccumulative (Section 3.6).

Findings that were found to have a robust weight of evidence supporting them had one or more highquality studies that were largely in agreement with each other. Findings that were said to have a moderate weight of evidence were based on a mix of high and medium-quality studies that were largely in agreement but varied in sample size and consistency of findings.

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APPENDICES 1326

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EPI SUITETM MODEL OUTPUT Appendix A

A.1 Melting Point, Boiling Point, and Vapor Pressure (MPBPVP)

```
1329
1330
         Run Date: 2024-06-12.
1331
1332
         Experimental Database Structure Match:
1333
                      : DICYCLOHEXYL PHTHALATE
: 000084-61-7
1334
            CAS Num
1335
            Exp MP (deg C):
                                  66
1336
            Exp BP (deg C):
                                  224 @ 4 mm Hq
                                 8.69E-07 (extrapolated)
1.16E-004
1337
            Exp VP (mm Hg):
1338
                     (Pa ):
1339
            Exp VP (deg C):
                                 25
1340
            Exp VP ref
                             : WERNER, AC (1952)
1341
1342
         SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3
         CHEM : Dicyclohexyl Phthalate MOL FOR: C20 H26 O4
1343
1344
1345
         MOL WT : 330.43
1346
         ------ SUMMARY MPBPWIN v1.44 ------------
1347
1348
1349
         Boiling Point: 394.85 deg C (Adapted Stein and Brown Method)
1350
1351
         Melting Point: 50.36 deg C (Adapted Joback Method)
Melting Point: 116.89 deg C (Gold and Ogle Method)
Mean Melt Pt: 83.63 deg C (Joback; Gold,Ogle Methods)
Selected MP: 61.45 deg C (Weighted Value)
1353
1354
1355
1356
         Vapor Pressure Estimations (25 deg C):
   (Using BP: 394.85 deg C (estimated))
1357
            (Using MP: 66.00 deg C (exp database))
VP: 1.07E-006 mm Hg (Antoine Method)
1358
1359
                    0.000142 Pa (Antoine Method)
4.58E-006 mm Hg (Modified Grain Method)
0.00061 Pa (Modified Grain Method)
1360
1361
1362
1363
                    8.93E-006 mm Hg (Mackay Method)
           : 0.00119 Pa (Mackay Method)

Selected VP: 4.58E-006 mm Hg (Modified Grain Method)

: 0.00061 Pa (Modified Grain Method)
1364
1365
1366
           Subcooled liquid VP: 2.21E-006 mm Hg (25 deg C, exp database VP)
: 0.000295 Pa (25 deg C, exp database VP)
1367
1368
1369
1370
1371
          TYPE | NUM | BOIL DESCRIPTION | COEFF | VALUE
          Group | 10 | -CH2- (ring)
Group | 2 | >CH- (ring)
Group | 2 | -COO- (ester)
                                                       26.44 |
21.66 |
78.85 |
1373
                                                                         264.40
1374
                                                                          43.32
1375
                                                                          157.70
                                                         28.53
30.76
1376
          Group | 4
                           | CH (aromatic)
                                                                          114.12
                           -C (aromatic)
1377
1378
                     2
          Group |
                                                                          61.52
                                                          -35.00
          Corr
                              Diester-type
                                                                          -35.00
1379
                  | | Equation Constant |
                                                                         198.18
1380
1381
         RESULT-uncorr | BOILING POINT in deg Kelvin | 804.24 RESULT- corr | BOILING POINT in deg Kelvin | 668.01
1382
                           | BOILING POINT in deg C | 394.85
1383
1384
1385
```

TYPE | NUM | MELT DESCRIPTION | COEFF | VALUE

December 2024

1 4 X X		L 			L
1388 1389 1390 1391 1392 1393 1394 1395	Group Group Group Group Group Corr	10 2 2 4 2 1	-CH2- (ring) >CH- (ring) -COO- (ester) CH (aromatic) -C (aromatic) Diester-type Equation Constant	7.75 19.88 53.60 8.13 37.02 -130.00	77.50 39.76 107.20 32.52 74.04 -130.00 122.50
1396 1397 1398	RESUI	=====- _T	+=====================================		+=====================================
1399					

A.2 Water Solubility

1200

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Two separate EPI SuiteTM models were used to estimate water solubility: WSKOWWIN and WATERNT. WSKOWWIN estimates water solubility using the selected K_{OW} and melting point values selected in Section (A.2.1). WATERNT estimates water solubility based on a quantitative structure activity relationship (QSAR) (A.2.2).

A.2.1 Water Solubility (WSKOWWIN)

```
Run Date: 2024-06-12.
1408
1409
1410
                            Water Sol: 1.48 mg/L
1411
1412
       Experimental Water Solubility Database Match:
1413
          Name
                       DICYCLOHEXYL PHTHALATE
1414
          CAS Num :
                       000084-61-7
         Exp WSol : 4 mg/L (24 deg C)
Exp Ref : YALKOWSKY,SH & DANNENFELSER,RM (1992)
1415
1416
       SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3
1419
               : Dicyclohexyl Phthalate
       CHEM
1420
       MOL FOR: C20 H26 O4
1421
       MOL WT : 330.43
                                 ----- WSKOW v1.43 Results -----
       Log Kow (estimated): 6.20
Log Kow (experimental): not available from database
1423
       Log Kow used by Water solubility estimates: 4.82 (user entered)
1426
1427
       Equation Used to Make Water Sol estimate:
           Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction
              Melting Pt (Tm) = 66.00 \text{ deg C (Use } Tm = 25 \text{ for all liquids})
1431
              Correction(s):
                                        Value
               No Applicable Correction Factors
1435
           Log Water Solubility (in moles/L) : -5.349 Water Solubility at 25 deg C (mg/L): 1.48
1438
1439
```

A.2.2 Water Solubility (WATERNT)

```
Run Date: 2024-06-12.

1442
1443
1444
1445
1445
1446

Run Date: 2024-06-12.

Water Sol (v1.01 est): 2.4027 mg/L

Water Solubility Database Match:

Name : DICYCLOHEXYL PHTHALATE
```

December 2024

CAS Num : 000084-61-7 Exp WSol : 4 mg/L (24 deg C) Exp Ref : YALKOWSKY,SH & DANNENFELSER,RM (1992)

SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3

CHEM : Dicyclohexyl Phthalate

MOL FOR: C20 H26 O4 MOL WT : 330.43

1473

			_ 1	
TYPE	NUM	WATER SOLUBILITY FRAGMENT DESCRIPTION	COEFF	VALUE
Frag Frag Frag Frag Const	2 4 2 2 10	-CH [aliphatic carbon] Aromatic Carbon (C-H type) -C(=0)0 [ester, aromatic attach] Aromatic Carbon (C-substituent type) -CH2- [aliphatic carbon, cyclic] Equation Constant	-0.5285 -0.3359 0.7006 -0.5400 -0.3308	-1.0570 -1.3435 1.4012 -1.0799 -3.3084 0.2492

Log Water Sol (moles/L) at 25 dec C = -5.1384 Water Solubility (mg/L) at 25 dec C = 2.4027

A.3 $Log K_{OW} (KOWWIN)$

Run Date: 2024-06-12.

Log Kow(version 1.69 estimate): 6.20

SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3

CHEM: Dicyclohexyl Phthalate MOL FOR: C20 H26 O4 MOL WT: 330.43

TYPE | NUM | LOGKOW FRAGMENT DESCRIPTION | COEFF | VALUE
 Frag
 10
 -CH2 [aliphatic carbon]
 0.4911
 4.9110

 Frag
 2
 -CH
 [aliphatic carbon]
 0.3614
 0.7228

 Frag
 6
 Aromatic Carbon
 0.2940
 1.7640

 Frag
 2
 -C(=0)0
 [ester, aromatic attach]
 -0.7121
 -1.4242

 Const
 Equation Constant
 0.2290
 Log Kow = 6.2026

A.4 Log K_{OA} (KOAWIN)

Run Date: 2024-06-12.

Log Koa: 10.23

SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3

CHEM : Dicyclohexyl Phthalate

MOL FOR: C20 H26 O4 MOL WT : 330.43

------ KOAWIN v1.10 Results ------

Log Koa (octanol/air) estimate: 10.233 Koa (octanol/air) estimate: 1.71e+010

Using:

Log Kow: 4.82 (user entered)

HenryLC: 9.45e-008 atm-m3/mole (user entered) Log Kaw: -5.413 (air/water part.coef.)

LogKow : --- (exp database) LogKow : 6.20 (KowWin estimate)

Henry LC: 1e-007 atm-m3/mole (exp database)

```
PUBLIC RELEASE DRAFT
                                                   December 2024
         Henry LC: 7.39e-007 atm-m3/mole (HenryWin bond estimate)
1509
1510
1511
         Log Koa (octanol/air) estimate: 10.720 (from KowWin/HenryWin)
1512
1513
        A.5 Henry's Log (HENRYWIN)
1514
        Run Date: 2024-06-12.
1515
1516
1517
1518
                Bond Est: 7.39E-007 atm-m3/mole (7.49E-002 Pa-m3/mole)
Group Est: 6.43E-008 atm-m3/mole (6.52E-003 Pa-m3/mole)
1519
1520
        SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3
1521
        CHEM : Dicyclohexyl Phthalate
        MOL FOR: C20 H26 O4
1523
        MOL WT : 330.43
        Experimental Database Structure Match:
        Name : DICYCLOHEXYL PHTHALATE

CAS Num : 000084-61-7

Exp HLC : 1.00E-07 atm-m3/mole (0.0101 Pa-m3/mole)

Temper : 25 deg C

Exp Ref : VP/WSOL
        CLASS | BOND CONTRIBUTION DESCRIPTION | COMMENT | VALUE
        HYDROGEN | 22 Hydrogen to Carbon (aliphatic) Bonds |
HYDROGEN | 4 Hydrogen to Carbon (aromatic) Bonds |
FRAGMENT | 12 C-C |
FRAGMENT | 2 C-O |
FRAGMENT | 6 Car-Car |
FRAGMENT | 2 Car-CO |
FRAGMENT | 2 CO-O |
                                                                                      | -2.6329
                                                                                       -0.6172
1535
                                                                                         1.3956
2.1709
1536
1538
                                                                                         1.5828
1539
                                                                                         2.4775
1540
                                                                                       0.1429
         RESULT | BOND ESTIMATION METHOD for LWAPC VALUE | TOTAL | 4.520
1541
1542
1543
       HENRYS LAW CONSTANT at 25 deg C = 7.39E-007 atm-m3/mole = 3.02E-005 unitless = 7.49E-002 Pa-m3/mole
1544
1545
            GROUP CONTRIBUTION DESCRIPTION COMMENT VALUE
                            10 CH2 (C)(C)
2 CH (C)(C)(O)
4 Car-H (Car)(Car)
1550
                                                                                            0.24
                                                                                            0.44
                            2 Car (Car)(Car)(C0)
2 CO (0)(Car)
2 O (C)(C0)
1553
                                                                                          | -1.68
                                                                                         9.14
1555
1556
1557
         RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | TOTAL | 5.58
1558
1559
        HENRYS LAW CONSTANT at 25 deg C = 6.43E-008 atm-m3/mole
                                          = 2.63E-006 unitless
1560
1561
                                             = 6.52E-003 Pa-m3/mole
1562
        A.6 K_{OC} (KOCWIN)
1563
        Run Date: 2024-06-12.
1564
1565
```

1566 SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3 1567 CHEM : Dicyclohexyl Phthalate MOL FOR: C20 H26 O4 MOL WT : 330.43 1568 1569

1570 ------ KOCWIN v2.01 Results ------

First Order Molecular Connectivity Index
Section Sect
Estimated Koc: 1.332e+004 L/kg <====================================
Koc Estimate from Log Kow: Log Kow (User entered)
Log Kow (User entered)
Fragment Correction(s): 2 Ester (-C-CO-O-C-) or (HCO-O-C) : -0.1312 Corrected Log Koc : 3.4600 Estimated Koc: 2884 L/kg <====================================
Corrected Log Koc : 3.4600 Estimated Koc: 2884 L/kg <=========== A.7 Hydrolysis Degradation Rate (HYDROWIN) Run Date: 2024-06-18 SMILES : C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3 CHEM : Dicyclohexyl Phthalate MOL FOR: C20 H26 04
A.7 Hydrolysis Degradation Rate (HYDROWIN) Run Date: 2024-06-18 SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3 CHEM: Dicyclohexyl Phthalate MOL FOR: C20 H26 O4
A.7 Hydrolysis Degradation Rate (HYDROWIN) Run Date: 2024-06-18 SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3 CHEM: Dicyclohexyl Phthalate MOL FOR: C20 H26 04
A.7 Hydrolysis Degradation Rate (HYDROWIN) Run Date: 2024-06-18 SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3 CHEM: Dicyclohexyl Phthalate MOL FOR: C20 H26 O4
Run Date: 2024-06-18 SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3 CHEM: Dicyclohexyl Phthalate MOL FOR: C20 H26 O4
Run Date: 2024-06-18 SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3 CHEM: Dicyclohexyl Phthalate MOL FOR: C20 H26 O4
CHEM : Dicyclohexyl Phthalate MOL FOR: C20 H26 O4
NOTE: Fragment(s) on this compound are NOT available from the fragment library. Substitute(s) have been used!!! Substitute R1, R2, R3, or R4 fragments are marked with double astericks "**".
ESTER: R1-C(=0)-0-R2 ** R1: -Phenyl
R2: -cyclohexyl NOTE: Ortho-position fragments(s) on Phenyl ring(s) are NOT CONSIDERED!! Kb hydrolysis at atom # 8: 9.417E-003 L/mol-sec
ESTER: R1-C(=0)-0-R2 R1: -Phenyl
R2: -cyclohexyl Kb hydrolysis at atom # 16: 9.417E-003 L/mol-sec
Total Kb for pH > 8 at 25 deg C : 1.883E-002 L/mol-sec Kb Half-Life at pH 8: 1.166 years Kb Half-Life at pH 7: 11.662 years
A.8 Tier III Fugacity (LEV3EpiTM)
The EPI Suite TM Fugacity Tier III model was run for four scenarios: 1000 kg/hr release to air, 1
kg/hr release to water, 1000 kg/hr release to soil, 1000 kg/hr release to all compartments (air, v soil).

soil). 1626

A.8.1 Release to Air

1628 Run Date: 2024-06-21

December 2024 CAS Number: 000084-61-7 1632 SMILES: 0=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCCC3)C3)c2 CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT: 330.43 ----- EPI SUMMARY (v4.11) ------Physical Property Inputs: Log Kow (octanol-water): 4.82 Boiling Point (deg C): 225.00

Melting Point (deg C): 66.00

Vapor Pressure (mm Hg): 8.69E-007

Water Solubility (mg/L): 1.48

Henry LC (atm-m3/mole): 9.446E-008 KOWWIN Program (v1.68) Results: Log Kow(version 1.69 estimate): 6.20 SMILES : O=C(OC(CCC1)C1)c(c(cc2)C(=0)OC(CCC3)C3)c2 CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43 1652 1653 TYPE | NUM | LOGKOW FRAGMENT DESCRIPTION | COEFF | VALUE -+----

 Frag
 10
 -CH2- [aliphatic carbon]
 0.4911
 4.9110

 Frag
 2
 -CH [aliphatic carbon]
 0.3614
 0.7228

 Frag
 6
 Aromatic Carbon
 0.2940
 1.7640

 Frag
 2
 -C(=0)0 [ester, aromatic attach]
 -0.7121
 -1.4242

 Const
 Equation Constant
 0.2290

 1659 Log Kow = 6.2026MPBPVP (v1.43) Program Results: Experimental Database Structure Match: Name : DICYCLOHEXYL PHTHALATE CAS Num : 000084-61-7 1671 Exp MP (deg C): 66
Exp BP (deg C): 224 @ 4 mm Hg
Exp VP (mm Hg): 8.69E-07 (extrapolated) 1.16E-004 (Pa): Exp VP (deg C): 25 Exp VP ref : WERNER, AC (1952) 1679 SMILES: 0=C(OC(CCC1)C1)c(c(ccc2)C(=0)OC(CCC3)C3)c2 CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43 ----- SUMMARY MPBPWIN v1.44 ------Boiling Point: 394.85 deg C (Adapted Stein and Brown Method) Melting Point: 50.36 deg C (Adapted Joback Method)
Melting Point: 116.89 deg C (Gold and Ogle Method)
Mean Melt Pt: 83.63 deg C (Joback; Gold,Ogle Methods)
Selected MP: 61.45 deg C (Weighted Value) Vapor Pressure Estimations (25 deg C): (Using BP: 225.00 deg C (user entered)) (Using MP: 66.00 deg C (user entered)) VP: 0.0445 mm Hg (Antoine Method)

December 2024

```
1697
                     5.93 Pa (Antoine Method)
1698
1699
               1700
                     0.0632 mm Hg (Mackay Method)
1701
                     8.43 Pa (Mackay Method)
            Selected VP: 0.0392 mm Hg (Modified Grain Method)
1702
1703
                               5.22 Pa (Modified Grain Method)
            Subcooled liquid VP: 2.21E-006 mm Hg (25 deg C, user-entered VP)
: 0.000295 Pa (25 deg C, user-entered VP)
1704
1705
1706
1707
1708
           TYPE | NUM | BOIL DESCRIPTION | COEFF | VALUE
1709
          -----+----+-----

        Group
        10
        -CH2- (ring)
        26.44
        264.40

        Group
        2
        >CH- (ring)
        21.66
        43.32

        Group
        2
        -C00- (ester)
        78.85
        157.70

        Group
        4
        CH (aromatic)
        28.53
        114.12

        Group
        2
        -C (aromatic)
        30.76
        61.52

        Corr
        1
        Diester-type
        -35.00
        -35.00

        *
        Equation Constant
        198.18

1710
1711
1712
1713
1714
1715
1716
1717
         RESULT-uncorr | BOILING POINT in deg Kelvin | 804.24
RESULT- corr | BOILING POINT in deg Kelvin | 668.01
BOILING POINT in deg C | 394.85
1718
1719
1720
1721
17\overline{2}
\overline{1723}
          -----+----+------
1724
          TYPE | NUM | MELT DESCRIPTION | COEFF | VALUE
1725
1726
1727
          ----+---+----
          1728
1729
1730
1731
\bar{1}7\bar{3}\bar{2}
1733
         _____+__+__+___+
1734
1735
1736
1737
             RESULT | MELTING POINT in deg Kelvin | 323.52
| MELTING POINT in deg C | 50.36
1738
1739
1740
         Water Sol from Kow (WSKOW v1.42) Results:
1741
         _____
1742
1743
                       Water Sol: 1.48 mg/L
1744
1745
         Experimental Water Solubility Database Match:
1746
1747
            Name : DICYCLOHEXYL PHTHALATE
CAS Num : 000084-61-7
Exp WSol : 4 mg/L (24 deg C)
Exp Ref : YALKOWSKY,SH & DANNENFELSER,RM (1992)
1748
1749
1750
1751
         SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
1752
         CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
         MOL FOR: C20 H26 O4 MOL WT : 330.43
1753
1754
1755
1756
1757
1758
1759
                                        Log Kow (estimated): 6.20
Log Kow (experimental): not available from database
Log Kow used by Water solubility estimates: 4.82 (user entered)
1760
         Equation Used to Make Water Sol estimate:
1761
              Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction
1762
```

Melting Pt (Tm) = 66.00 deg C (Use Tm = 25 for all liquids)

December 2024 1764 1765 1766 Correction(s): Value 1767 No Applicable Correction Factors 1768 Log Water Solubility (in moles/L): -5.349 Water Solubility at 25 deg C (mg/L): 1.48 1769 1770 1771 1772 1773 1774 1775 WATERNT Program (v1.01) Results: _____ 1776 water Sol (v1.01 est): 2.4027 mg/L 1778 1779 Experimental Water Solubility Database Match: : DICYCLOHEXYL PHTHALATE 1780 CAS Num : 000084-61-7 Exp WSol : 4 mg/L (24 deg C) 1781 1782 1783 Exp Ref : YALKOWSKY, SH & DANNENFELSER, RM (1992) 1784 1785 SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 178<u>6</u> 1787 1788 MOL WT : 330.43 1789 1790 TYPE | NUM | WATER SOLUBILITY FRAGMENT DESCRIPTION | COEFF | VALUE 1791 -----Frag | 2 | -CH [aliphatic carbon]
Frag | 4 | Aromatic Carbon (C-H type)
Frag | 2 | -C(=0)0 [ester, aromatic attach]
Frag | 2 | Aromatic Carbon (C-substituent type)
Frag | 10 | -CH2- [aliphatic carbon, cyclic]
Const | Equation Constant 1792 -CH [aliphatic carbon] | -1.0570 | -1.3435 |-0.5285 |-0.3359 -1.3435 1.4012 1793 1794 0.7006 1795 | -1.0799 | -3.3084 |-0.5400 1796 0.3308 1797 0.2492 1798 1799 Log Water Sol (moles/L) at 25 dec C = -5.13841800 water Solubility (mg/L) at 25 dec C = 1801 1802 1803 1804 ECOSAR Program (v1.11) Results: 1805 1806 ECOSAR Version 1.11 Results Page 1807 1808 SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCCC3)C3)c21809 CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester 1810 CAS Num: 1811 ChemID1: 1812 MOL FOR: C20 H26 O4 MOL WT : 330.43 Log Kow: 6.203 (EpiSuite Kowwin v1.68 Estimate) 1815 Log Kow: (User Entered) (PhysProp DB exp value - for comparison only) 1816 Log Kow: (deg C, User Entered for Wat Sol estimate) Melt Pt: 66.00 1817 Melt Pt: 66.00 (deg C, PhysProp DB exp value for Wat Sol est) 1818 (mg/L, EpiSuite WSKowwin v1.43 Estimate) 1819 Wat Sol: 0.06964 1820 1821 1822 1823 1824 1825 (mg/L, User Entered) Wat Sol: 1.48 (mg/L, PhysProp DB exp value) Wat Sol: 4 _____ Values used to Generate ECOSAR Profile 1826 Log Kow: 6.203 (EpiSuite Kowwin v1.68 Estimate) Wat Sol: 1.48 (mg/L, User Entered) 1828

1833

_____ Esters

ECOSAR v1.11 Class-specific Estimations

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
	 Fish	96-hr	LC50	0.155
	: Daphnid_	48-hr	LC50	0.206
	Green Algae	96-hr	EC50	0.045
	: Fish		ChV	0.005
	: Daphnid		ChV	0.042
	Green Algae		ChV	0.045
Esters :	: Fish (SW)	96-hr	LC50	0.183
	: Mysid	96-hr	LC50	0.023
	: Fish (SW)		ChV	0.056
Esters :	Mysid (SW)		ChV	0.000318
Esters :	Earthworm	14-day	LC50	190.265 *
=======================================	==========	======	=====	=======
	Fish	96-hr	LC50	0.046
(Baseline Toxicity) :	: Daphnid	48-hr	LC50	0.038
:	Green Algae	96-hr	EC50	0.142
:	: Fish		ChV	0.007
:	: Daphnid		ChV	0.011
:	: Green Algae		ChV	0.088

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10x, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Esters:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)

Maximum LogKow: 6.0 (Earthworm LC50) Maximum LogKow: 6.4 (Green Algae EC50)

Maximum LogKow: 8.0 (ChV)

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50) Maximum LogKow: 6.4 (Green Algae EC50) Maximum LogKow: 8.0 (ChV)

HENRYWIN (v3.20) Program Results:

Bond Est: 7.39E-007 atm-m3/mole (7.49E-002 Pa-m3/mole) Group Est: 6.43E-008 atm-m3/mole (6.52E-003 Pa-m3/mole)

SMILES: 0=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCCC3)C3)c2CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

MOL FOR: C20 H26 O4 MOL WT : 330.43

December 2024

```
1898
        ------ HENRYWIN v3.21 Results ------
1899
1900
        Experimental Database Structure Match:
          Name : DICYCLOHEXYL PHTHALATE

CAS Num : 000084-61-7

Exp HLC : 1.00E-07 atm-m3/mole (0.0101 Pa-m3/mole)

Temper : 25 deg C

Exp Ref : VP/WSOL
1901
1902
1903
1904
1905
1906
1907
        CLASS | BOND CONTRIBUTION DESCRIPTION | COMMENT | VALUE

HYDROGEN | 22 Hydrogen to Carbon (aliphatic) Bonds | -2.6329

HYDROGEN | 4 Hydrogen to Carbon (aromatic) Bonds | -0.6172

FRAGMENT | 12 C-C | 1.3956

FRAGMENT | 2 C-O | 2.1709

FRAGMENT | 6 Car-Car | 1.5828

FRAGMENT | 2 Car-CO | 2.4775

FRAGMENT | 2 CO-O | 0.1429
1908
1909
1910
1913
1914
1915
1916
1917
1918
         RESULT | BOND ESTIMATION METHOD for LWAPC VALUE | TOTAL | 4.520
1919
        HENRYS LAW CONSTANT at 25 deg C = 7.39E-007 atm-m3/mole = 3.02E-005 unitless
1920
1921
1922
                                              = 7.49E-002 Pa-m3/mole
1923
1924
                         _____
         GROUP CONTRIBUTION DESCRIPTION | COMMENT | VALUE
1925
1926
1927
        10 CH2 (C)(C)
2 CH (C)(C)(0)
4 Car-H (Car)(Car)
2 Car (Car)(Car)(C0)
2 CO (O)(Car)
                                                                                  | -1.50
                                                                                         0.24
0.44
-1.68
9.14
1931
                      2 0 (c)(co)
1934
         RESULT | GROUP ESTIMATION METHOD for LOG GAMMA VALUE | TOTAL | 5.58
1935
       HENRYS LAW CONSTANT at 25 deg C = 6.43E-008 atm-m3/mole = 2.63E-006 unitless = 6.52E-003 Pa-m3/mole
1936
1937
1938
1939
1940
1941
        For Henry LC Comparison Purposes:
          Exper Database: 1.00E-07 atm-m3/mole (1.01E-002 Pa-m3/mole)
User-Entered Henry LC: 9.446E-008 atm-m3/mole (9.571E-003 Pa-m3/mole)
1942
1943
          Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 2.553E-007 atm-m3/mole (2.587E-002 Pa-m3/mole)
VP: 8.69E-007 mm Hg (source: User-Entered)
1944
1945
1946
1947
                     1.48 mg/L (source: User-Entered)
             WS:
1948
1949
1950
        Log Octanol-Air (KOAWIN v1.10) Results:
1951
1952
        1953
1954
                  Log Koa: 10.233
1955
       SMILES : 0=C(OC(CCC1)C1)c(c(cc2)C(=0)OC(CCC3)C3)c2 CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4
1956
1957
1958
1959
        MOL WT : 330.43
1960
                   1961
1962
        Log Koa (octanol/air) estimate: 10.233
1963
            Koa (octanol/air) estimate: 1.711e+010
1964
         Using:
```

December 2024 Log Kow: 4.82 (user entered)
HenryLC: 9.45e-008 atm-m3/mole (user entered)
Log Kaw: -5.413 (air/water part.coef.) LogKow : ---- (exp database) LogKow : 6.20 (KowWin estimate) Henry LC: 1e-007 atm-m3/mole (exp database) Henry LC: 7.39e-007 atm-m3/mole (HenryWin bond estimate) Log Koa (octanol/air) estimate: 10.720 (from KowWin/HenryWin) 1976 BIOWIN (v4.10) Program Results: SMILES : 0=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCCC3)C3)c2 CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43 Biowin1 (Linear Model Prediction) : Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months
Biowin4 (Primary Biodegradation Timeframe): Days
Biowin5 (MITI Linear Model Prediction) : Biodegrades Fast
Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast
Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast Ready Biodegradability Prediction: NO 2002 2003 TYPE | NUM | Biowin2 FRAGMENT DESCRIPTION | COEFF | VALUE Frag | 2 | Ester [-C(=0)-O-C] | 4.0795 | 8.1590 MolWt| * | Molecular Weight Parameter | -4.6921 _____+ 2012 RESULT | Biowin2 (Non-Linear Biodeg Probability) | | 0.9985 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast TYPE | NUM | Biowin3 FRAGMENT DESCRIPTION | COEFF | VALUE

Frag | 2 | Ester [-C(=0)-O-C] | 0.1402 | 0.2804

Molwt| * | Molecular Weight Parameter | -0.7302

Const | * | Equation Constant | 3.1992 RESULT | Biowin3 (Survey Model - Ultimate Biodeg) | 2.7494 ______ TYPE | NUM | Biowin4 FRAGMENT DESCRIPTION | COEFF | VALUE

Frag | 2 | Ester [-C(=0)-O-C] | 0.2290 | 0.4579

MolWt| * | Molecular Weight Parameter | -0.4767

	مد ا	December 2024			
Const	* ======	Equation Constant	=======	3.8477 +=======	
RESULT Biowin4 (Survey Model - Primary Biodeg)				3.8289	
Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> wee (Primary & Ultimate) 2.00 -> months 1.00 -> longer					
TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag Frag Frag Frag MolWt Const	:	Ester [-C(=0)-O-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Molecular Weight Parameter Equation Constant	0.4638 0.0016 0.1411 0.0158 -0.5211 0.5544		
RESU	ULT	Biowin5 (MITI Linear Biodeg Probability)		0.6556	
	+	+========+++		+======= +	
TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag Frag Frag Frag MolWt	2 4 10 2 *	Ester [-C(=0)-O-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Molecular Weight Parameter	1.5833 0.0342 0.1206 0.0294	3.1665 0.1368 1.2058 0.0589 -5.7164	
RES	ULT			0.6257	

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag Frag Frag Frag Const	2 4 10 2	Ester [-C(=0)-O-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Equation Constant	0.1719 -0.0954 -0.1200 0.0395	0.3437 -0.3817 -1.2001 0.0789 0.8361
RESU	JLT	Biowin7 (Anaerobic Linear Biodeg Prob)	+======= -========	-0.3232

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

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```
2099
       BioHCwin (v1.01) Program Results:
2100
2101
       SMILES: 0=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCCC3)C3)c2
2102
              : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
2103
       MOL FOR: C20 H26 O4
2104
       MOL WT : 330.43
2105
                     ----- BioHCwin v1.01 Results ------
2106
2107
2108
         NO Estimate Possible ... Structure NOT a Hydrocarbon
            (Contains atoms other than C, H or S (-S-))
2109
2110
2112
2113
       AEROWIN Program (v1.00) Results:
2114
        Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
         Vapor pressure (liquid/subcooled): 0.000295 Pa (2.21E-006 mm Hq)
2115
2116
2117
         Log Koa (Koawin est ): 10.233
          Kp (particle/gas partition coef. (m3/ug)):
2118
2119
          Mackay model : 0.0102
Octanol/air (Koa) model: 0.0042
Fraction sorbed to airborne particulates (phi):
2120
2121
2122
               Junge-Pankow model
                                          0.269
                                          0.449
               Mackay model
\bar{2}1\bar{2}\bar{3}
               Octanol/air (Koa) model: 0.251
2124
2124
2125
2126
2127
2128
2129
       AOP Program (v1.92) Results:
       SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
       CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
2130
2131
       MOL FOR: C20 H26 O4 MOL WT : 330.43
\overline{2}\overline{1}\overline{3}\overline{2}
                     ----- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) ------
2133
                                = 23.5226 E-12 cm3/molecule-sec
       Hydrogen Abstraction
2134
2135
2136
2137
2138
       Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
       Addition to Triple Bonds
                                   = 0.0000 E-12 cm3/molecule-sec
       Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
       **Addition to Aromatic Rings = 0.7492 E-12 cm3/molecule-sec
       Addition to Fused Rings
                                       0.0000 E-12 cm3/molecule-sec
2139
2140
          OVERALL OH Rate Constant = 24.2718 E-12 cm3/molecule-sec
2141
                           0.441 Days (12-hr day; 1.5E6 OH/cm3)
          HALF-LIFE =
                          5.288 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
2142
          HALF-LIFE =
2143
       2144
       ----- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) ------
2145
2146
                       ***** NO OZONE REACTION ESTIMATION *****
\tilde{2}\tilde{1}4\tilde{7}
                       (ONLY Olefins and Acetylenes are Estimated)
2149
       Experimental Database: NO Structure Matches
2150
       Fraction sorbed to airborne particulates (phi):
2151
         0.359 (Junge-Pankow, Mackay avg)
2152
         0.251 (Koa method)
2153
            Note: the sorbed fraction may be resistant to atmospheric oxidation
2154
2155
2156
\bar{2}157
2158
       KOCWIN Program (v2.00) Results:
2159
2160
       SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
2161
       CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
2162
       MOL FOR: C20 H26 O4
2163
       MOL WT : 330.43
2164
              ----- KOCWIN v2.01 Results -----
```

 $\overline{2}\overline{1}65$

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2166

2167 2168

2169 2170

 $\bar{2}\bar{1}71$

2172

2173 2174 2175

2176 2177

2187 2188 2189

2190 2191

2197 2198

2199

2200

2201 2202

2203

 $\bar{2}\bar{2}\bar{0}4$

2205 2206 2207

2208

2209

2210 2211

 $\bar{2}\bar{2}15$

2218

```
Koc Estimate from MCI:
         First Order Molecular Connectivity Index .....: 11.737
Non-Corrected Log Koc (0.5213 MCI + 0.60) .....: 6.7184
         Fragment Correction(s):
                     Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -2.5939
         Corrected Log Koc .....: 4.1245
                          Estimated Koc: 1.332e+004 L/kg <========
  Koc Estimate from Log Kow:
         Log Kow (User entered
         Non-Corrected Log Koc (0.55313 logKow + 0.9251) ...:
                                                                      3.5912
         Fragment Correction(s):
                   2 Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -0.1312
         Corrected Log Koc .....: 3.4600
                          Estimated Koc: 2884 L/kg <=======
HYDROWIN Program (v2.00) Results:
SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
              ----- HYDROWIN v2.00 Results -----
NOTE: Fragment(s) on this compound are NOT available from the fragment
    library. Substitute(s) have been used!!! Substitute R1, R2, R3,
    or R4 fragments are marked with double astericks "**"
                                       ** R1: -Phenyl
ESTER: R1-C(=0)-0-R2
                                          R2: -cyclohexyl
NOTE: Ortho-position fragments(s) on Phenyl ring(s) are NOT CONSIDERED!! Kb hydrolysis at atom # 2: 9.417E-003 L/mol-sec
ESTER: R1-C(=0)-0-R2
                                          R1: -Phenyl
                                          R2: -cyclohexyl
 Kb hydrolysis at atom # 15: 9.417E-003 L/mol-sec
 Total Kb for pH > 8 at 25 deg C : 1.883E-002 L/mol-sec
Kb Half-Life at pH 8: 1.166 years
Kb Half-Life at pH 7: 11.662 years
BCFBAF Program (v3.01) Results:
SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
     : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4 MOL WT : 330.43
               -----BCFBAF v3.01 ------
Summary Results:
 Log BCF (regression-based estimate): 2.85 (BCF = 703 L/kg wet-wt)
Biotransformation Half-Life (days): 0.159 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 1.83 (BAF = 67.1 L/kg wet-wt)
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 4.82 (user entered)
```

```
Equation Used to Make BCF estimate:
Log BCF = 0.6598 log Kow - 0.333 + Correction
```

Correction(s): Value
No Applicable Correction Factors

Estimated Log BCF = 2.847 (BCF = 703.5 L/kg wet-wt)

Whole Body Primary Biotransformation Rate Estimate for Fish:

Whole Body Primary Biotransformation Rate Estimate for Fish:

TYPE	NUM	LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION	COEFF	VALUE
Frag Frag Frag Frag Frag Frag Molwt Const	2 4 10 2 1 * *	Ester [-C(=0)-O-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Benzene Log Kow = 4.82 (user-entered) Molecular Weight Parameter Equation Constant	-0.7605 0.2664 0.0963 0.0126 -0.4277 0.3073	-1.5211 1.0655 0.9625 0.0252 -0.4277 1.4814 -0.8473 -1.5371
RESU RESU NOTE	LT į	LOG Bio Half-Life (days) Bio Half-Life (days) Bio Half-Life (days) Bio Half-Life Normalized to 10 g fish at 15	-=====================================	 -0.7986 0.159

Biotransformation Rate Constant:

kM (Rate Constant): 4.359 /day (10 gram fish)
kM (Rate Constant): 2.451 /day (100 gram fish)
kM (Rate Constant): 1.378 /day (1 kg fish)
kM (Rate Constant): 0.7752 /day (10 kg fish)

Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates): Estimated Log BCF (upper trophic) = 1.827 (BCF = 67.13 L/kg wet-wt) Estimated Log BAF (upper trophic) = 1.827 (BAF = 67.13 L/kg wet-wt) Estimated Log BCF (mid trophic) = 1.959 (BCF = 90.99 L/kg wet-wt) Estimated Log BAF (mid trophic) = 1.962 (BAF = 91.63 L/kg wet-wt) Estimated Log BCF (lower trophic) = 1.999 (BCF = 99.71 L/kg wet-wt) Estimated Log BAF (lower trophic) = 2.031 (BAF = 107.3 L/kg wet-wt)

Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 3.758 (BCF = 5725 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 4.731 (BAF = 5.377e+004 L/kg wet-wt)

Volatilization From Water

Chemical Name: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

Molecular Weight : 330.43 g/mole water Solubility : 1.48 ppm Vapor Pressure : 8.69E-007 mm Hg

Henry's Law Constant: 9.45E-008 atm-m3/mole (entered by user)

HALF-LIFE (hours): 1.127E+004 1.231E+005

December 2024

2300

2300 2301 2302

2303 2304

2305

2306

 $\bar{2}314$

2315

2316

2324 2325

2331 2332 2333

2340 2341

2342 2343

2344

2349

2350

2351

2352 2353

2354

2359

2360

2361

 $\bar{2}362$

2363

2364 2365

2366

-Aeration tank

```
469.5
      HALF-LIFE (days):
                                              5129
      HALF-LIFE (years):
                            1.286
                                              14.04
STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
                              _____
   (using 10000 \text{ hr Bio P,A,S})
PROPERTIES OF: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
                                                       330.43
Molecular weight (g/mol)
Aqueous solubility (mg/l)
                                                       1.48
Vapour pressure (Pa)
                                                       0.000115857
                (atm)
                                                       1.14342E-009
                (mm Hg)
                                                       8.69E-007
                                                       9.446E-008
Henry 's law constant (Atm-m3/mol)
Air-water partition coefficient
                                                       3.86313E-006
Octanol-water partition coefficient (Kow)
                                                       66069.4
                                                       4.82
Biomass to water partition coefficient
                                                       13214.7
Temperature [deg C]
                                                       25
Biodeg rate constants (h^-1), half life in biomass (h) and in 2000 mg/L MLSS (h):

-Primary tank 0.00 9635.43 10000.00
                                         9635.43
          -Primary tank
-Aeration tank
                                                       10000.00
                               0.00
                                         9635.43
          -Settling tank
                                         9635.43
                               0.00
                                                       10000.00
 STP Overall Chemical Mass Balance:
 -----
                             g/h
                                               mol/h
                                                              percent
Influent
                            1.00E+001
                                              3.0E-002
                                                              100.00
Primary sludge
Waste sludge
                            4.35E+000
                                              1.3E-002
                                                              43.54
                                              8.2E-003
                            2.70E+000
                                                              27.02
Primary volatilization
                            1.41E-005
                                              4.3E-008
                                                              0.00
Settling volatilization
                            3.44E-005
                                              1.0E-007
                                                               0.00
Aeration off gas
                            8.47E-005
                                              2.6E-007
                                                               0.00
Primary biodegradation
                            1.32E-002
                                              4.0E-005
                                                               0.13
Settling biodegradation
                            3.53E-003
                                              1.1E-005
                                                               0.04
Aeration biodegradation
                            4.65E-002
                                              1.4E-004
                                                               0.47
Final water effluent
                            2.88E+000
                                              8.7E-003
                                                              28.81
Total removal
                            7.12E+000
                                              2.2E-002
                                                              71.19
Total biodegradation
                            6.32E-002
                                              1.9E-004
                                                               0.63
STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
      _____
   (using Biowin/EPA draft method)
PROPERTIES OF: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
Molecular weight (g/mol)
                                                       330.43
Aqueous solubility (mq/l)
                                                       1.48
Vapour pressure (Pa)
                                                       0.000115857
                                                       1.14342E-009
                (atm)
                (mm Hg)
                                                       8.69E-007
Henry 's law constant (Atm-m3/mol)
                                                       9.446E-008
Air-water partition coefficient
                                                       3.86313E-006
Octanol-water partition coefficient (Kow)
                                                       66069.4
Log Kow
                                                       4.82
Biomass to water partition coefficient
                                                       13214.7
Temperature [deg C]
                                                       25
Biodeg rate constants (h^-1), half life in biomass (h) and in 2000 mg/L MLSS (h):
                              0.01
                                                         100.00
          -Primary tank
                                           96.35
```

9.64

10.00

0.07

2367

2368 **2**369

2370 2371

 $\bar{2}\bar{3}72$ 2373

2374

2380 2381

2388

2389

2390 2391 $\bar{2}392$

 $\bar{2}397$ 2398 $\bar{2}399$

2400

2401

2402 2403

2404

2405

2406

2407

2408

2409 2410

2411

2412

2413 2414

2415

2416

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2420

2421

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2429

2430

2431

Sediment

1.85

December 2024 -Settling tank 0.07 9.64 10.00 STP Overall Chemical Mass Balance: g/h mol/h percent Influent 1.00E+001 3.0E-002 100.00 Primary sludge 3.85E+0001.2E-002 38.51 2.37E-001 7.2E-004 Waste sludge 2.37 Primary volatilization 3.8E-008 1.25E-005 0.00 3.02E-006 Settling volatilization 9.1E-009 0.00 Aeration off gas 7.61E-006 2.3E-008 0.00 Primary biodegradation 1.17E+000 3.5E-003 11.68 3.10E-001 9.4E-004 3.10 Settling biodegradation Aeration biodegradation 4.18E+000 1.3E-002 41.81 Final water effluent 2.53E-001 7.7E-004 2.53 Total removal 9.75E+0002.9E-002 97.47 Total biodegradation 5.66E+000 1.7E-002 56.59 (** Total removal recommended maximum is 95 percent) Level III Fugacity Model (Full-Output): MCI Method Chem Name : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester Molecular Wt: 330.43 Henry's LC: 9.45e-008 atm-m3/mole (user-entered) Vapor Press: 8.69e-007 mm Hg (user-entered) Liquid VP: 2.21e-006 mm Hg (super-cooled) : 66 deg C (user-entered) Melting Pt : 4.82 (user-entered) Log Kow Soil Koc : 1.33e+004 (KOCWIN MCI method) Half-Life Mass Amount Emissions (percent) (hr) (kg/hr) Air 1.43 10.6 1000 2.41 900 0 Water Soil 94.3 1.8e+003 0 1.85 8.1e+003 0 Sediment Fugacity Reaction Advection Reaction Advection (kg/hr) (percent) (atm) (kg/hr) (percent) 5.05e-012 96.1 Air 630 63 9.61 2.26e-014 Water 12.5 16.2 1.25 1.62 3.15e-014 244 0 24.4 0 Soil Sediment 2.78e-014 1.07 0.249 0.107 0.0249 Persistence Time: 672 hr 757 hr Reaction Time: Advection Time: 5.97e+003 hr Percent Reacted: 88.7 Percent Advected: 11.3 Water Compartment Percents: Mass Amount Half-Life **Emissions** (percent) (hr) (kg/hr) 1.43 Air 10.6 1000 Water 2.41 900 0 (2.35)water (0.00778)biota suspended sediment (0.047) 94.3 1.8e+003 Soil 0

0

8.1e+003

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```
2434
          Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin): Air: 10.58
2435
<del>2</del>436
                         900
              Water:
                         1800
              Soil:
              Sediment: 8100
2440
                Biowin estimate: 2.749 (weeks-months)
2441
          Advection Times (hr):
2443
              Air:
                         100
2444
              Water:
                         1000
2445
              Sediment: 5e+004
2446
2447
2448
       Level III Fugacity Model (Full-Output): EQC Default
2449
2450
         Chem Name
                     : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
2451
         Molecular Wt: 330.43
2452
                      : 9.45e-008 atm-m3/mole (user-entered)
         Henry's LC
2453
         Vapor Press: 8.69e-007 mm Hg (user-entered)
2454
         Liquid VP
                       : 2.21e-006 mm Hg (super-cooled)
                      : 66 deg C (user-entered)
2455
         Melting Pt
2456
                       : 4.82 (user-entered)
         Log Kow
2457
         Soil Koc
                       : 2.71e+004 (EQC Model Default)
2458
2459
                                    Half-Life
                   Mass Amount
                                                  Emissions
2460
                     (percent)
                                       (hr)
                                                    (kg/hr)
2461
                                                      1000
          Air
                      1.41
                                       10.6
2462
          Water
                      2.25
                                       900
                                                      0
2463
                      92.9
                                       1.8e + 003
                                                      0
          Soil
2464
          Sediment
                     3.47
                                       8.1e+003
                                                      0
2465
2466
                                   Reaction
                                                Advection
                                                                           Advection
                      Fugacity
                                                             Reaction
2467
                       (atm)
                                   (kg/hr)
                                                 (kg/hr)
                                                              (percent)
                                                                           (percent)
                                                 96.1
2468
          Air
                      5.05e-012
                                    630
                                                               63
                                                                            9.61
2469
          Water
                      2.11e-014
                                    11.8
                                                 15.4
                                                               1.18
                                                                            1.54
2470
                      1.55e-014
                                    244
                                                 0
                                                               24.4
                                                                            0
          Soil
                                    2.03
2471
                                                 0.474
                                                               0.203
                                                                            0.0474
          Sediment
                     2.6e-014
2473
          Persistence Time: 683 hr
2474
                              769 hr
          Reaction Time:
2475
          Advection Time:
                              6.1e+003 hr
2476
                              88.8
          Percent Reacted:
2477
          Percent Advected: 11.2
2478
2479
          Water Compartment Percents:
2480
2481
                                    Half-Life
                                                  Emissions
                   Mass Amount
                     (percent)
                                       (hr)
                                                    (kg/hr)
          Air
                      1.41
                                       10.6
                                                      1000
                      2.25
                                                      0
                                       900
          Water
2485
                        (2.16)
            water
2486
                        (0.00712)
             biota
2487
             suspended sediment (0.0876)
2488
                                       1.8e + 003
                                                      0
                     92.9
2489
          Sediment 3.47
                                       8.1e+003
                                                      0
2490
          Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin): Air: 10.58
2491
2492
2493
                         900
              Water:
2494
              Soil:
                         1800
2495
              Sediment: 8100
2496
                Biowin estimate: 2.749 (weeks-months)
2497
2498
          Advection Times (hr):
                         100
2499
              Air:
2500
              Water:
                         1000
```

2501 Sediment: 5e+004

```
2502
              A.8.2 Release to Water
2503
       Run Date: 2024-06-21
2504
```

2505

2506

2507 2508

 $\frac{2509}{2509}$

2510

2511 2512

2513

2514

2515

2516

2517

 $\overline{2518}$

2520

2526 2527 2528

 $\bar{2529}$ 2530

2541 2542

2543 2544

2545

2546

2547

2548

2549

2550 2551

2552

2553 2554

2555 2556

2560 2561

2563

2564 2565 CAS Number: 000084-61-7

SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

MOL FOR: C20 H26 O4

MOL WT : 330.43

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

Physical Property Inputs:

Log Kow (octanol-water): 4.82 Boiling Point (deg C) : 225.00 Melting Point (deg C) : Vapor Pressure (mm Hg) : 66.00 8.69E-007 Water Solubility (mg/L): 1.48 Henry LC (atm-m3/mole): 9.446E-008

KOWWIN Program (v1.68) Results:

Log Kow(version 1.69 estimate): 6.20

SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

MOL FOR: C20 H26 O4 MOL WT : 330.43

		·		1
TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag Frag Frag Frag Const	10 2 6 2	-CH2- [aliphatic carbon] -CH [aliphatic carbon] Aromatic Carbon -C(=0)0 [ester, aromatic attach] Equation Constant	0.4911 0.3614 0.2940 -0.7121	4.9110 0.7228 1.7640 -1.4242 0.2290
_	F	-	Log Kow =	6.2026

MPBPVP (v1.43) Program Results:

Experimental Database Structure Match:

: DICYCLOHEXYL PHTHALATE Name : 000084-61-7

CAS Num Exp MP (deg C): Exp BP (deg C): 66

224 @ 4 mm Hg

Exp VP (mm Hg): (Pa): 8.69E-07 (extrapolated)

1.16E-004

Exp VP (deg C): 25

Exp VP ref WERNER, AC (1952)

SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4

MOL WT : 330.43 ----- SUMMARY MPBPWIN v1.44 -----

Boiling Point: 394.85 deg C (Adapted Stein and Brown Method)

Melting Point: 50.36 deg C (Adapted Joback Method) Melting Point: 116.89 deg C (Gold and Ogle Method)
Mean Melt Pt: 83.63 deg C (Joback; Gold, Ogle Methods)

PUBLIC RELEASE DRAFT December 2024 Selected MP: 61.45 deg C (Weighted Value) 2568 Vapor Pressure Estimations (25 deg C):
(Using BP: 225.00 deg C (user entered))
(Using MP: 66.00 deg C (user entered))
VP: 0.0445 mm Hg (Antoine Method) 2569 5.93 Pa (Antoine Method) VP: 0.0392 mm Hg (Modified Grain Method)
 : 5.22 Pa (Modified Grain Method) : 5.22 Pa (MODITIEU GRAIN MELHOU)
VP: 0.0632 mm Hg (Mackay Method)
: 8.43 Pa (Mackay Method)
Selected VP: 0.0392 mm Hg (Modified Grain Method)
: 5.22 Pa (Modified Grain Method)
Subcooled liquid VP: 2.21E-006 mm Hg (25 deg C, user-entered VP)
: 0.000295 Pa (25 deg C, user-entered VP) 2577 ______ TYPE | NUM | BOIL DESCRIPTION | COEFF | VALUE Group | 10 | -CH2- (ring) | 26.44 | 264.40 Group | 2 | >CH- (ring) | 21.66 | 43.32 Group | 2 | -COO- (ester) | 78.85 | 157.70 Group | 4 | CH (aromatic) | 28.53 | 114.12 Group | 2 | -C (aromatic) | 30.76 | 61.52 Corr | 1 | Diester-type | -35.00 | -35.00 * | Equation Constant | 198.18 2587 2588 RESULT-uncorr| BOILING POINT in deg Kelvin | 804.24 RESULT- corr | BOILING POINT in deg Kelvin | 668.01 | BOILING POINT in deg C | 394.85 595 2596 TYPE | NUM | MELT DESCRIPTION | COEFF | VALUE $\frac{2603}{2604}$ RESULT | MELTING POINT in deg Kelvin | 323.52 | MELTING POINT in deg C | 50.36 2614 Water Sol from Kow (WSKOW v1.42) Results: _____ Water Sol: 1.48 mg/L Experimental Water Solubility Database Match: Name : DICYCLOHEXYL PHTHALATE
CAS Num : 000084-61-7
Exp WSol : 4 mg/L (24 deg C) Exp Ref : YALKOWSKY, SH & DANNENFELSER, RM (1992) 2627 SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43

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Log Kow (estimated): 6.20 Log Kow (experimental): not available from database

December 2024 2633 Log Kow used by Water solubility estimates: 4.82 (user entered) 2634 **2**635 Equation Used to Make Water Sol estimate: 2636 Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction2637 2638 Melting Pt (Tm) = 66.00 deg C (Use Tm = 25 for all liquids)2639 2640 Correction(s): Value 2641 2642 No Applicable Correction Factors 2643 Log Water Solubility (in moles/L): -5.349 Water Solubility at 25 deg C (mg/L): 2647 2648 2649 WATERNT Program (v1.01) Results: 2650 2651 2652 water Sol (v1.01 est): 2.4027 mg/L 2653 2654 Experimental Water Solubility Database Match: DICYCLOHEXYL PHTHALATE 2655 Name 2656 000084-61-7 CAS Num 2657 Exp WSol : 4 mg/L (24 deg C) 2658 Exp Ref : YALKOWSKY, SH & DANNENFELSER, RM (1992) 2659 2660 SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 2661 $\frac{2661}{2662}$ 2663 MOL WT : 330.43 2664 2665 TYPE | NUM | WATER SOLUBILITY FRAGMENT DESCRIPTION | COEFF | VALUE 2666 |-0.5285 2667 Frag | | -CH [aliphatic carbon] -1.0570 Aromatic Carbon (C-H type) 2668 Frag 4 |-0.3359 -1.34352669 2 -C(=0)0 [ester, aromatic attach] | 0.7006 1.4012 Frag | Aromatic Carbon (C-substituent type) 2670 2 Frag | |-0.5400 -1.079910 2671 -CH2- [aliphatic carbon, cyclic] -0.3308-3.3084 Frag 2672 Const | Equation Constant 0.2492 2673 2674 Log Water Sol (moles/L) at 25 dec C = Water Solubility (mg/L) at 25 dec C = -5.1384 2675 2.4027 2676 2677 2678 2679 ECOSAR Program (v1.11) Results: 2680 2681 ECOSAR Version 1.11 Results Page 2682 2683 SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c22684 : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester CHEM 2685 CAS Num: 2686 ChemID1: 2687 MOL FOR: C20 H26 O4 2688 MOL WT : 330.43 Log Kow: 6.203 Log Kow: Log Kow: 2689 (EpiSuite Kowwin v1.68 Estimate) 2690 (User Entered) (PhysProp DB exp value - for comparison only) (deg C, User Entered for Wat Sol estimate) (deg C, PhysProp DB exp value for Wat Sol est) 2691 2692 Melt Pt: 66.00 2693 Melt Pt: 66.00 2694 wat Sol: 0.06964 (mg/L, EpiSuite WSKowwin v1.43 Estimate) (mg/L, User Entered) 2695 Wat Sol: 1.48

2696

2697 2698 2699 Wat Sol: 4

(mg/L, PhysProp DB exp value)

December 2024

```
Values used to Generate ECOSAR Profile
```

Log Kow: 6.203 (EpiSuite Kowwin v1.68 Estimate) Wat Sol: 1.48 (mg/L, User Entered)

ECOSAR v1.11 Class-specific Estimations

Esters

2700

2701 2702

2708

2709 2710

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ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Esters	: Fish	96-hr	LC50	0.155
Esters	: Daphnid	48-hr	LC50	0.206
Esters	: Green Algae	96-hr	EC50	0.045
Esters	: Fish		ChV	0.005
Esters	: Daphnid_		ChV	0.042
Esters	: Green Algae		ChV	0.045
Esters	: Fish (SW)	96-hr	LC50	0.183
Esters	: Mysid	96-hr	LC50	0.023
Esters	: Fish (SW)		ChV	0.056
Esters	: Mysid (SW) : Earthworm	14 day	ChV	0.000318 190.265 *
Esters	. Ear Chworm	14-day	LC50	190.203 "
		=======	======	========
Neutral Organic SAR	: Fish	96-hr	LC50	0.046
(Baseline Toxicity)	: Daphnid	48-hr	LC50	0.038
·	: Green Algae	96-hr	EC50	0.142
	: Fish		ChV	0.007
	: Daphnid		ChV	0.011
	: Green Algae		ChV	0.088

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES)

are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Esters:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)

Maximum LogKow: 6.0 (Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50) Maximum LogKow: 6.4 (Green Algae EC50) Maximum LogKow: 8.0 (ChV)

HENRYWIN (v3.20) Program Results:

Bond Est: 7.39E-007 atm-m3/mole (7.49E-002 Pa-m3/mole)

December 2024

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Group Est: 6.43E-008 atm-m3/mole (6.52E-003 Pa-m3/mole)
```

SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

MOL FOR: C20 H26 O4 MOL WT : 330.43

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28082809 2810

2815

------- HENRYWIN v3.21 Results -----------

Experimental Database Structure Match: : DICYCLOHEXYL PHTHALATE

CAS Num : 000084-61-7 Exp HLC : 1.00E-07 atm-m3/mole (0.0101 Pa-m3/mole) Temper : 25 deg C Exp Ref : VP/WSOL

CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN HYDROGEN FRAGMENT FRAGMENT FRAGMENT FRAGMENT FRAGMENT	22 Hydrogen to Carbon (aliphatic) Bonds 4 Hydrogen to Carbon (aromatic) Bonds 12 C-C 2 C-O 6 Car-Car 2 Car-CO 2 CO-O		-2.6329 -0.6172 1.3956 2.1709 1.5828 2.4775 0.1429
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	4.520
	I The state of the	, 7	1

HENRYS LAW CONSTANT at 25 deg C = 7.39E-007 atm-m3/mole = 3.02E-005 unitless = 7.49E-002 Pa-m3/mole

	l		I <i></i>
	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	10 CH2 (C)(C) 2 CH (C)(C)(0) 4 Car-H (Car)(Car) 2 Car (Car)(Car)(C0) 2 CO (0)(Car) 2 0 (C)(CO)		-1.50 0.24 0.44 -1.68 9.14 -1.06
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	5.58

HENRYS LAW CONSTANT at 25 deg C = 6.43E-008 atm-m3/mole = 2.63E-006 unitless = 6.52E-003 Pa-m3/mole

For Henry LC Comparison Purposes:

Exper Database: 1.00E-07 atm-m3/mole (1.01E-002 Pa-m3/mole)
User-Entered Henry LC: 9.446E-008 atm-m3/mole (9.571E-003 Pa-m3/mole)
Henrys LC [via VP/WSol estimate using USer-Entered (male)]:

HLC: 2.553E-007 atm-m3/mole (2.587E-002 Pa-m3/mole) VP: 8.69E-007 mm Hg (source: User-Entered)

WS: 1.48 mg/L (source: User-Entered)

Log Octanol-Air (KOAWIN v1.10) Results:

Log Koa: 10.233

SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

MOL FOR: C20 H26 O4

December 2024 2834 MOL WT : 330.43 2835 2836 Log Koa (octanol/air) estimate: 10.233 Koa (octanol/air) estimate: 1.711e+010 Using: Log Kow: 4.82 (user entered) HenryLC: 9.45e-008 atm-m3/mole (user entered) Log Kaw: -5.413 (air/water part.coef.) 2843 LogKow : --- (exp database)
LogKow : 6.20 (KowWin estimate)
Henry LC: 1e-007 atm-m3/mole (exp database)
Henry LC: 7.39e-007 atm-m3/mole (HenryWin bond estimate) Log Koa (octanol/air) estimate: 10.720 (from KowWin/HenryWin) 2852 2853 BIOWIN (v4.10) Program Results: SMILES: O=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCCC3)C3)c2
CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4 2855 2856 2857 2858 MOL WT : 330.43 2859 -----BIOWIN v4.10 Results ------2860 Biowin1 (Linear Model Prediction) : Biodegrades Fast
Biowin2 (Non-Linear Model Prediction): Biodegrades Fast
Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months
Biowin4 (Primary Biodegradation Timeframe): Days
Biowin5 (MITI Linear Model Prediction) : Biodegrades Fast
Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast
Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast 2862 2863 2864 2865 2866 2867 2868 Ready Biodegradability Prediction: NO 2869 2870 ______ TYPE | NUM | Biowin1 FRAGMENT DESCRIPTION | COEFF | VALUE Frag | 2 | Ester [-C(=0)-O-C] | 0.1742 | 0.3484 | Molwt| * | Molecular Weight Parameter | -0.1573 | Const | * | Equation Constant | 0.7475 2873 2874 2875 2876 RESULT | Biowin1 (Linear Biodeg Probability) | 0.9386 2877 2878 2880 TYPE | NUM | Biowin2 FRAGMENT DESCRIPTION | COEFF | VALUE 2881 Frag | 2 | Ester [-C(=0)-0-C] | 4.0795 | 8.1590 | MolWt| * | Molecular Weight Parameter | -4.6921 2885 RESULT | Biowin2 (Non-Linear Biodeg Probability) | 0.9985 2886 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast 2890 2891 2892 2893 TYPE | NUM | Biowin3 FRAGMENT DESCRIPTION | COEFF | VALUE 2894 ----+-----Frag | 2 | Ester [-C(=0)-O-C] | 0.1402 | 0.2804 MolWt| * | Molecular Weight Parameter | -0.7302 Const| * | Equation Constant | 3.1992 2895 2896 2898 RESULT | Biowin3 (Survey Model - Ultimate Biodeg) | 2.7494 2899 2900

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TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag MolWt Const	2 * *	Ester [-C(=0)-O-C] Molecular Weight Parameter Equation Constant	0.2290	0.4579 -0.4767 3.8477
RESU	JLT	Biowin4 (Survey Model - Primary Biodeg)		3.8289
Result (Prin	Class	sification: 5.00 -> hours 4.00 -> days Ultimate) 2.00 -> months 1.00 -> longer	3.00 ->	weeks
TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag Frag Frag Frag MolWt Const	2 4 10 2 *	Ester [-C(=0)-O-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Molecular Weight Parameter Equation Constant	0.2319 0.0004 0.0141 0.0079	0.4638 0.0016 0.1411 0.0158 -0.5211 0.5544
RESU	JLT		-======	0.6556
				r=====================================
TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag Frag Frag Frag MolWt	2 4 10 2 *	Ester [-C(=0)-O-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Molecular Weight Parameter	1.5833 0.0342 0.1206 0.0294	3.1665 0.1368 1.2058 0.0589 -5.7164

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable A Probability Less Than 0.5 indicates --> NOT Readily Degradable

RESULT | Biowin6 (MITI Non-Linear Biodeg Probability) | 0.6257

TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag Frag Frag Frag Const	2 4 10 2 *	Ester [-C(=0)-O-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Equation Constant	0.1719 -0.0954 -0.1200 0.0395	0.3437 -0.3817 -1.2001 0.0789 0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)	-======= 	-0.3232

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for

December 2024

degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

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2996

2997

 $\frac{1}{2}$ 998

2999 3000 3001

3002 3003

3004

3005

3006

3012 3013

3014 3015

3016

3020

3023 3024

3025

3026 3027 3028

3034

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BioHCwin (v1.01) Program Results:
_____
SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4 MOL WT : 330.43
             ----- BioHCwin v1.01 Results -----
  NO Estimate Possible ... Structure NOT a Hydrocarbon
    (Contains atoms other than C, H or S (-S-))
AEROWIN Program (v1.00) Results:
 Sorption to aerosols (25 Dec C)[AEROWIN v1.00]: Vapor pressure (liquid/subcooled): 0.000295 Pa (2.21E-006 mm Hg)
  Log Koa (Koawin est ): 10.233
   Kp (particle/gas partition coef. (m3/ug)):
                                 0.0102
       Mackay model
       Octanol/air (Koa) model: 0.0042
   Fraction sorbed to airborne particulates (phi):
                             : 0.269
       Junge-Pankow model
       Mackay_model
                                 0.449
       Octanol/air (Koa) model: 0.251
AOP Program (v1.92) Results:
SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
      : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
Hydrogen Abstraction = 23.5226 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings = 0.7492 E-12 cm3/molecule-sec
                          = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings
   OVERALL OH Rate Constant = 24.2718 E-12 cm3/molecule-sec
***** NO OZONE REACTION ESTIMATION *****
               (ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi):
  0.359 (Junge-Pankow, Mackay avg) 0.251 (Koa method)
     Note: the sorbed fraction may be resistant to atmospheric oxidation
KOCWIN Program (v2.00) Results:
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3035
      SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
      CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43
3036
3037
3038
3039
               ------ KOCWIN v2.01 Results ------
3040
3041
        Koc Estimate from MCI:
3042
3043
               First Order Molecular Connectivity Index .....: 11.737
               Non-Corrected Log Koc (0.5213 MCI + 0.60) ...... : 6.7184
3044
3045
               Fragment Correction(s):
3046
                           Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -2.5939
3047
               Corrected Log Koc ..... 4.1245
3049
                               Estimated Koc: 1.332e+004 L/kg <========
3050
3051
        Koc Estimate from Log Kow:
3052
3053
               Log Kow (User entered
               Non-Corrected Log Koc (0.55313 logKow + 0.9251) ....: 3.5912
3054
3055
               Fragment Correction(s):
3056
                            Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -0.1312
3057
               Corrected Log Koc
3058
3059
                               Estimated Koc: 2884 L/kg <=======
3060
3061
3062
3063
3064
      HYDROWIN Program (v2.00) Results:
3065
3066
      SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
3067
            : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
3068
      MOL FOR: C20 H26 O4
3069
      MOL WT : 330.43
                    3070
3071
3072
3073
      NOTE: Fragment(s) on this compound are NOT available from the fragment
          library. Substitute(s) have been used!!! Substitute R1, R2, R3, or R4 fragments are marked with double astericks "**".
3074
3075
3076
3077
                                           ** R1: -Phenyl
      ESTER: R1-C(=0)-0-R2
3078
                                              R2: -cyclohexyl
       NOTE: Ortho-position fragments(s) on Phenyl ring(s) are NOT CONSIDERED!!
3079
3080
       Kb hydrolysis at atom # 2: 9.417E-003 L/mol-sec
3081
3082
      ESTER: R1-C(=0)-0-R2
                                              R1: -Phenyl
3083
                                              R2: -cyclohexyl
3084
       Kb hydrolysis at atom # 15: 9.417E-003 L/mol-sec
3085
3086
       Total Kb for pH > 8 at 25 deg C : 1.883E-002 L/mol-sec
       Kb Half-Life at pH 8:
                                  1.166 years
3087
3088
       Kb Half-Life at рн 7:
                                  11.662 years
3089
3090
3091
3092
3093
      BCFBAF Program (v3.01) Results:
3094
3095
      SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
      CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4
3096
3097
3098
      MOL WT : 330.43
3099
                    ----- BCFBAF v3.01 ------
3100
      Summary Results:
3101
        Log BCF (regression-based estimate): 2.85 (BCF = 703 L/kg wet-wt)
```

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December 2024
   Biotransformation Half-Life (days): 0.159 (normalized to 10 g fish) Log BAF (Arnot-Gobas upper trophic): 1.83 (BAF = 67.1 \text{ L/kg wet-wt})
Log Kow (experimental): not available from database
Log Kow used by BCF estimates: 4.82 (user entered)
Equation Used to Make BCF estimate:
    Log BCF = 0.6598 log Kow - 0.333 + Correction
         Correction(s):
                                                              value
          No Applicable Correction Factors
    Estimated Log BCF = 2.847 (BCF = 703.5 L/kg wet-wt)
          ______
Whole Body Primary Biotransformation Rate Estimate for Fish:
TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
 Frag | 2 | Ester [-C(=0)-O-C]
Frag | 4 | Aromatic-H
Frag | 10 | -CH2- [cyclic]
Frag | 2 | -CH - [cyclic]
Frag | 1 | Benzene
L Kow * | Log Kow = 4.82 (user-entered
MolWt * | Molecular Weight Parameter
Const | * | Equation Constant
                                                                                          -0.7605 | -1.5211
0.2664 | 1.0655
0.0963 | 0.9625
                                                                                           0.0126 | 0.0252
                                                                                          -0.4277 | -0.4277
                                                                                          0.3073 | 1.4814
                                                                                                        0.8473
                                                                                                        | -1.5371
RESULT
    RESULT | LOG Bio Half-Life (days) | | RESULT | Bio Half-Life (days) | | NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C
                                                                                                          -0.7986
                                                                                                         0.159
Biotransformation Rate Constant:
 kM (Rate Constant): 4.359 /day (10 gram fish)
kM (Rate Constant): 2.451 /day (100 gram fish)
kM (Rate Constant): 1.378 /day (1 kg fish)
kM (Rate Constant): 0.7752 /day (10 kg fish)
Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
    Estimated Log BCF (upper trophic) = 1.827 (BCF = 67.13 L/kg wet-wt)
    Estimated Log BAF (upper trophic) = 1.827 (BAF = 67.13 L/kg wet-wt)
    Estimated Log BCF (mid trophic) = 1.959 (BCF = 90.99 L/kg wet-wt)
    Estimated Log BAF (mid trophic) = 1.962 (BAF = 91.63 L/kg wet-wt)
    Estimated Log BCF (lower trophic) = 1.999 (BCF = 99.71 L/kg wet-wt)
    Estimated Log BAF (lower trophic) = 2.031 (BAF = 107.3 L/kg wet-wt)
Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
Estimated Log BCF (upper trophic) = 3.758 (BCF = 5725 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 4.731 (BAF = 5.377e+004 L/kg wet-wt)
                                           Volatilization From Water
                                           Chemical Name: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
Molecular Weight
                                   330.43 g/mole
Water Solubility : 1.48 ppm
Vapor Pressure : 8.69E-007 mm Hg
```

RIVER LAKE

Henry's Law Constant: 9.45E-008 atm-m3/mole (entered by user)

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3169
3170
3171
        Water Depth
Wind Velocity (meters):
(m/sec):
                                              5
                                                                     0.5
3172
         Current Velocity (m/sec):
                                             1
                                                                     0.05
3173
3174
                HALF-LIFE (hours) : 1.127E+004
HALF-LIFE (days) : 469.5
HALF-LIFE (years) : 1.286
                                                                   1.231E+005
3175
                                                                    5129
3176
                                                                     14.04
3177
3178
3179
3180
         STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
         ______
3181
         (using 10000 hr Bio P,A,S)
3182
3183
         PROPERTIES OF: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
3184
                                                                                 330.43
         Molecular weight (g/mol)
3185
         Aqueous solubility (mg/l)
                                                                                 1.48
3186
         Vapour pressure (Pa)
                                                                                 0.000115857
3187
                                                                                 1.14342E-009
                              (atm)
3188
3189
                              (mm Hg)
                                                                                 8.69E-007
                                                                                9.446E-008
3.86313E-006
         Henry 's law constant (Atm-m3/mol)
3190
         Air-water partition coefficient
3191
3192
         Octanol-water partition coefficient (Kow)
                                                                                66069.4
         Log Kow
                                                                                 4.82
3193
         Biomass to water partition coefficient
                                                                                 13214.7
3194
         Temperature [deg C]
                                                                                 25
3195
         Biodeg rate constants (h^-1), half life in biomass (h) and in 2000 mg/L MLSS (h):
                     -Primary tank 0.00 9635.43 10000.00

-Aeration tank 0.00 9635.43 10000.00

-Settling tank 0.00 9635.43 10000.00
3196
3197
3198
                     -Settling tank
3199
3200
          STP Overall Chemical Mass Balance:
3201
3202
                                                                    mol/h
                                                                                          percent
3203
3204
         Influent
                                             1.00E+001
                                                                   3.0E-002
                                                                                          100.00
3205

      Primary sludge
      4.35E+000
      1.3E-002
      43.54

      Waste sludge
      2.70E+000
      8.2E-003
      27.02

      Primary volatilization
      1.41E-005
      4.3E-008
      0.00

      Settling volatilization
      3.44E-005
      1.0E-007
      0.00

      Aeration off gas
      8.47E-005
      2.6E-007
      0.00

3206
3207
3\overline{208}
3209
3210
3211
        Primary biodegradation 1.32E-002
Settling biodegradation 3.53E-003
Aeration biodegradation 4.65E-002
3212
                                                                    4.0E-005
1.1E-005
1.4E-004
                                                                                          0.13
\bar{3}\bar{2}\bar{1}\bar{3}
                                                                                           0.04
3214
                                                                                           0.47
3215
3216
3217
         Final water effluent
                                             2.88E+000
                                                                    8.7E-003
                                                                                          28.81
         Total removal
         Total removal 7.12E+000 Total biodegradation 6.32E-002
                                                                     2.2E-002
1.9E-004
                                                                                           0.63
3220
3221
3222
3222
3223
         STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
3224
3225
3225
3226
3227
3228
                  _____
         (using Biowin/EPA draft method)
         PROPERTIES OF: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
         Molecular weight (g/mol)
Aqueous solubility (mg/l)
                                                                                 330.43
3229
                                                                                 1.48
3230
                                                                                 0.000115857
         Vapour pressure (Pa)
3231
                              (atm)
                                                                                 1.14342E-009
                              (mm Hq)
                                                                                8.69E-007
3233
         Henry 's law constant (Atm-m3/mol)
                                                                                9.446E-008
3234
                                                                                3.86313E-006
         Air-water partition coefficient
```

66069.4

Octanol-water partition coefficient (Kow)

```
December 2024
3236
       Log Kow
                                                                   4.82
3237
3238
3238
       Biomass to water partition coefficient
                                                                   13214.7
       Temperature [deg C]
                                                                   25
       Biodeg rate constants (h^-1), half life in biomass (h) and in 2000 mg/L MLSS (h):
3240
                  -Primary tank
                                     0.01
                                                                     100.00
                                                      96.35
                                         0.07
                                                       9.64
                  -Aeration tank
                                                                      10.00
                                                       9.64
                  -Settling tank
                                         0.07
                                                                      10.00
3243
3244
        STP Overall Chemical Mass Balance:
3245
3246
3247
                                                          mol/h
                                                                          percent
3248
       Influent
                                     1.00E+001
                                                         3.0E-002
                                                                          100.00
3249
3250
       Primary sludge
                                     3.85E+000
                                                         1.2E-002
                                                                           38.51
3251
       Waste sludge
                                     2.37E-001
                                                         7.2E-004
                                                                           2.37
       Primary volatilization
                                     1.25E-005
                                                         3.8E-008
                                                                           0.00
3253
                                                                           0.00
       Settling volatilization
                                     3.02E-006
                                                         9.1E-009
3254
3255
3256
3257
                                                         2.3E-008
                                     7.61E-006
                                                                           0.00
       Aeration off gas
                                     1.17E+000
       Primary biodegradation
                                                         3.5E-003
                                                                          11.68
                                                         9.4E-004
       Settling biodegradation
                                     3.10E-001
                                                                           3.10
3258
3259
       Aeration biodegradation
                                     4.18E+000
                                                         1.3E-002
                                                                           41.81
3260
       Final water effluent
                                                                           2.53
                                     2.53E-001
                                                         7.7E-004
3261
3262
                                                         2.9E-002
                                     9.75E+000
                                                                           97.47
       Total removal
3263
       Total biodegradation
                                     5.66E+000
                                                         1.7E-002
                                                                           56.59
3264
3265
        (** Total removal recommended maximum is 95 percent)
3266
3267
       Level III Fugacity Model (Full-Output): MCI Method
3268
3269
         Chem Name : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
3270
         Molecular Wt: 330.43
3271
         Henry's LC : 9.45e-008 atm-m3/mole (user-entered)
3272
         Vapor Press: 8.69e-007 mm Hg (user-entered)
3273
3274
         Liquid VP : 2.21e-006 mm Hg (super-cooled)
         Melting Pt
                     : 66 deg C (user-entered)
3\overline{275}
         Log_Kow : 4.82 (user-entered)
3276
3277
         Soil Koc
                     : 1.33e+004 (KOCWIN MCI method)
3278
                                   Half-Life
                   Mass Amount
                                                 Emissions
3279
                    (percent)
                                                   (kg/hr)
                                       (hr)
3280
          Air
                     0.000513
                                       10.6
3281
                                       900
                                                     1000
                     56.5
          Water
                     0.0338
                                       1.8e + 003
                                                     0
          Soil
          Sediment
                     43.5
                                       8.1e+003
                     Fugacity
                                  Reaction
                                               Advection
                                                            Reaction
                                                                         Advection
3286
                                  (kg/hr)
                                                (kg/hr)
                      (atm)
                                                             (percent)
                                                                          (percent)
                     2.58e-015
                                   0.321
                                                0.049
                                                             0.0321
                                                                           0.0049
          Air
3288
                     7.54e-013
          Water
                                   416
                                                540
                                                             41.6
                                                                          54
                                                             0.0124
                     1.6e-017
                                                0
                                                                          0
          Soil
                                   0.124
3290
                                                8.31
                                                                          0.831
          Sediment 9.25e-013
                                   35.5
                                                             3.55
3291
          Persistence Time: 956 hr
3293
                              2.12e+003 hr
          Reaction Time:
3\overline{2}94
          Advection Time:
                              1.74e+003 hr
3295
          Percent Reacted:
                              45.2
3296
          Percent Advected: 54.8
3297
3298
          Water Compartment Percents:
3299
3300
                                   Half-Life
                   Mass Amount
                                                  Emissions
3301
                                       (hr)
                                                   (kg/hr)
                    (percent)
3302
          Air
                     0.000513
                                       10.6
```

December 2024

```
3303
                                        900
           Water
                      56.5
                                                       1000
                        (55.2)
3304
             water
3305
                         (0.182)
             biota
3306
             suspended sediment (1.1)
3307
                                        1.8e+003
                                                       0
           Soil
                      0.0338
3308
           Sediment
                     43.5
                                        8.1e+003
                                                       0
3309
           Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin): Air: 10.58
3310
3311
3312
                         900
              Water:
3313
              soil:
                         1800
              Sediment: 8100
                 Biowin estimate: 2.749 (weeks-months)
3317
           Advection Times (hr):
3318
                         100
              Air:
              Water:
                         1000
3320
              Sediment: 5e+004
3321
3322
3323
3324
       Level III Fugacity Model (Full-Output): EQC Default
3325
3326
3327
          Chem Name : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
          Molecular Wt: 330.43
                       : 9.45e-008 atm-m3/mole (user-entered)
          Henry's LC
33\overline{28}
          Vapor Press: 8.69e-007 mm Hg (user-entered)
3329
                       : 2.21e-006 mm Hg (super-cooled)
          Liquid VP
3330
          Melting Pt
                       : 66 deg C (user-entered)
3331
3332
          Log Kow
                       : 4.82 (user-entered)
          Soil Koc
                       : 2.71e+004 (EQC Model Default)
                                     Half-Life
                    Mass Amount
                                                    Emissions
3335
                                        (hr)
                                                     (kg/hr)
                     (percent)
3336
                      0.00035
           Air
                                        10.6
                                                       0
3337
           Water
                      39.3
                                        900
                                                       1000
                                        1.8e+003
3338
                      0.0231
           Soil
                                                       0
3339
           Sediment
                                        8.1e+003
                                                       0
                      60.6
3340
3341
                      Fugacity
                                    Reaction
                                                 Advection
                                                               Reaction
                                                                            Advection
3342
                                    (kg/hr)
                                                  (kg/hr)
                       (atm)
                                                               (percent)
                                                                            (percent)
3343
           Air
                      2.42e-015
                                     0.301
                                                  0.046
                                                                0.0301
                                                                             0.0046
3344
                      7.08e-013
                                                                39.8
                                     398
           Water
                                                  517
                                                                             51.7
3345
           Soil
                      7.42e-018
                                                  0
                                                                0.0117
                                                                             0
                                     0.117
3346
           Sediment 8.75e-013
                                                  15.9
                                     68.2
                                                                6.82
                                                                             1.59
3347
3348
           Persistence Time: 1.31e+003 hr
<u>3349</u>
           Reaction Time:
                               2.82e+003 hr
3350
3351
3352
                               2.47e+003 hr
           Advection Time:
                               46.7
           Percent Reacted:
           Percent Advected: 53.3
3353
3354
           Water Compartment Percents:
3355
3356
                                     Half-Life
                    Mass Amount
                                                   Emissions
3357
                     (percent)
                                        (hr)
                                                     (kg/hr)
3358
           Air
                      0.00035
                                        10.6
3359
                      39.3
                                                       1000
                                        900
           Water
3360
                        (37.7)
             water
3361
             biota
                        (0.124)
3362
             suspended sediment (1.53)
3363
                                        1.8e + 003
           Soil
                      0.0231
                                                       0
3364
           Sediment 60.6
                                        8.1e+003
                                                       0
3365
3366
           Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
3367
                         10.58
3368
                         900
              Water:
```

3369

soil:

```
December 2024
3370
3371
3372
               Sediment: 8100
                  Biowin estimate: 2.749 (weeks-months)
3373
           Advection Times (hr):
                         100
3374
               Air:
3375
               Water:
                           1000
3376
               Sediment: 5e+004
3377
               A.8.3 Release to Soil
3378
        Run Date: 2024-06-21
3379
3380
        CAS Number: 000084-61-7
3381
3382
        SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
        CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
3383
        MOL FOR: C20 H26 O4
3384
        MOL WT : 330.43
3385
                 3386
3387
         Physical Property Inputs:
            Log Kow (octanol-water): 4.82
Boiling Point (deg C): 225.00
Melting Point (deg C): 66.00
Vapor Pressure (mm Hg): 8.69E-007
Water Solubility (mg/L): 1.48
Henry LC (atm-m3/mole): 9.446E-008
3388
3389
3390
3391
3392
3393
3394
3395
        KOWWIN Program (v1.68) Results:
3396
        _____
3397
3398
                            Log Kow(version 1.69 estimate): 6.20
3399
3400
        SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
3401
        CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
        MOL FOR: C20 H26 O4
3402
3403
        MOL WT : 330.43
3404
         TYPE | NUM | LOGKOW FRAGMENT DESCRIPTION | COEFF | VALUE
3405
3406

      Frag
      10
      -CH2-
      [aliphatic carbon]
      0.4911
      4.9110

      Frag
      2
      -CH
      [aliphatic carbon]
      0.3614
      0.7228

      Frag
      6
      Aromatic Carbon
      0.2940
      1.7640

      Frag
      2
      -C(=0)0
      [ester, aromatic attach]
      -0.7121
      -1.4242

      Const
      Equation Constant
      0.2290

3407
3408
3409
3410
3411
3412
3413
                                                                            Log Kow = 6.2026
3414
3415
3416
3417
        MPBPVP (v1.43) Program Results:
3418
              ------
3419
        Experimental Database Structure Match:
          Name : DICYCLOHEXYL PHTHALATE CAS Num : 000084-61-7
3420
3421
          Exp MP (deg C): 66
Exp BP (deg C): 224 @ 4 mm Hg
3423
          3424
34\bar{2}5
3429
        SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
3430
        CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
        MOL FOR: C20 H26 O4
3431
        MOL WT : 330.43
        ----- SUMMARY MPBPWIN v1.44 ------
```

```
December 2024
Boiling Point: 394.85 deg C (Adapted Stein and Brown Method)
                   50.36 deg C (Adapted Joback Method)
116.89 deg C (Gold and Ogle Method)
83.63 deg C (Joback; Gold,Ogle Methods)
61.45 deg C (Weighted Value)
Melting Point:
Melting Point:
Mean Melt Pt:
  Selected MP:
Vapor Pressure Estimations (25 deg C):
   (Using BP: 225.00 deg C (user entered))
   (Using MP: 66.00 deg C (user entered))
VP: 0.0445 mm Hg (Antoine Method)
         5.93 Pa (Antoine Method)
0.0392 mm Hg (Modified Grain Method)
5.22 Pa (Modified Grain Method)
         0.0632 mm Hg (Mackay Method)
       : 8.43 Pa (Mackay Method)
  Selected VP: 0.0392 mm Hg (Modified Grain Method)
: 5.22 Pa (Modified Grain Method)
  Subcooled liquid VP: 2.21E-006 mm Hg (25 deg C, user-entered VP)
: 0.000295 Pa (25 deg C, user-entered VP)
 TYPE | NUM | BOIL DESCRIPTION | COEFF | VALUE
-----+----+-----
 Group | 10 | -CH2- (ring) | 26.44 | 264.40
```

Group Group Group Group Corr	2 2 4 2 1	>CH- (ring) -COO- (ester) CH (aromatic) -C (aromatic) Diester-type Equation Constant	21.66 78.85 28.53 30.76 -35.00	204.40 43.32 157.70 114.12 61.52 -35.00 198.18
RESULT-		BOILING POINT in de BOILING POINT in de BOILING POINT in de	eg Kelvin	804.24 668.01 394.85
TYPE	+ NUM	MELT DESCRIPTION	+	VALUE
Group Group Group Group	10 2 2 4 4	-CH2- (ring) >CH- (ring) -COO- (ester) CH (aromatic) -C (aromatic)	7.75 19.88 53.60 8.13 37.02	77.50 39.76 107.20 32.52 74.04

Group | 2 | -C00- (ester) | 53.60 | 107.20 | Group | 4 | CH (aromatic) | 8.13 | 32.52 | Group | 2 | -C (aromatic) | 37.02 | 74.04 | Corr | 1 | Diester-type | -130.00 | -130.00 | | Equation Constant | 122.50 | | RESULT | MELTING POINT in deg Kelvin | 323.52 | MELTING POINT in deg C | 50.36

Water Sol from Kow (WSKOW v1.42) Results:

Water Sol: 1.48 mg/L

Experimental Water Solubility Database Match:

Name : DICYCLOHEXYL PHTHALATE

CAS Num : 000084-61-7

Exp WSol: 4 mg/L (24 deg C)

Exp Ref : YALKOWSKY, SH & DANNENFELSER, RM (1992)

SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2

```
December 2024
        CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43
3502
3503
3504
3505
                                    Log Kow (estimated): 6.20
Log Kow (experimental): not available from database
3506
3507
3508
        Log Kow used by Water solubility estimates: 4.82 (user entered)
3509
3510
        Equation Used to Make Water Sol estimate:
3511
            Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction
3512
3513
               Melting Pt (Tm) = 66.00 \text{ deg C (Use } Tm = 25 \text{ for all liquids})
3515
               Correction(s):
                                           Value
3517
                No Applicable Correction Factors
3518
           Log Water Solubility (in moles/L) : -5.349 Water Solubility at 25 deg C (mg/L): 1.48
3520
3521
3522
3523
3524
3525
        WATERNT Program (v1.01) Results:
        _____
3526
35\overline{27}
                             Water Sol (v1.01 est): 2.4027 mg/L
35\bar{2}8
3529
        Experimental Water Solubility Database Match:
          Name : DICYCLOHEXYL PHTHALATE
CAS Num : 000084-61-7
Exp WSol : 4 mg/L (24 deg C)
Exp Ref : YALKOWSKY,SH & DANNENFELSER,RM (1992)
3530
3531
3535
        SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
3536
               : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
3537
        MOL FOR: C20 H26 O4
3538
        MOL WT : 330.43
3539
3540
         TYPE | NUM | WATER SOLUBILITY FRAGMENT DESCRIPTION | COEFF | VALUE
3541
         Frag | 2 | -CH [aliphatic carbon]
Frag | 4 | Aromatic Carbon (C-H type)
Frag | 2 | -C(=0)0 [ester, aromatic attach]
Frag | 2 | Aromatic Carbon (C-substituent type)
Frag | 10 | -CH2- [aliphatic carbon, cyclic]
3542
                                                                               |-0.5285 | -1.0570
3543
                                                                               j-0.3359
                                                                                             | -1.3435
3544
                                                                               0.7006
                                                                                              1.4012
3545
                                                                               |-0.5400
                                                                                              -1.0799
3546
                                                                                1-0.3308
                                                                                              -3.3084
3547
                                                                                             0.2492
         Const
                      | Equation Constant
3548
                                            Log Water Sol (moles/L) at 25 dec C = -5.1384 Water Solubility (mg/L) at 25 dec C = 2.4027
3549
3550
3553
3554
        ECOSAR Program (v1.11) Results:
3555
3556
        ECOSAR Version 1.11 Results Page
3557
3558
        SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
3559
        CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
3560
        CAS Num:
3561
        ChemID1:
3562
        MOL FOR: C20 H26 O4
        MOL WT : 330.43
3563
        Log Kow: 6.203
3564
                                 (EpiSuite Kowwin v1.68 Estimate)
3565
        Log Kow:
                                (User Entered)
3566
        Log Kow:
                                (PhysProp DB exp value - for comparison only)
        Melt Pt: 66.00
                                 (deg C, User Entered for Wat Sol estimate)
3567
```

(deg C, PhysProp DB exp value for Wat Sol est)

3568

Melt Pt: 66.00

December 2024

```
3569
3570
3571
                                               (mg/L, EpiSuite WSKowwin v1.43 Estimate)
(mg/L, User Entered)
(mg/L, PhysProp DB exp value)
            Wat Sol: 0.06964
            wat Sol: 1.48 wat Sol: 4
3572
3573
```

Values used to Generate ECOSAR Profile -----

Log Kow: 6.203 (EpiSuite Kowwin v1.68 Estimate) Wat Sol: 1.48 (mg/L, User Entered)

ECOSAR v1.11 Class-specific Estimations

 $36\bar{2}\dot{2}$

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Esters	: Fish	96-hr	===== LC50	0.155
Esters	: Daphnid	48-hr	LC50	0.206
Esters	: Green Algae	96-hr	EC50	0.045
Esters	: Fish		ChV	0.005
Esters	: Daphnid_		ChV	0.042
Esters	: Green Algae		Chy	0.045
Esters	: Fish (SW)	96-hr	LC50	0.183
Esters	: Mysid	96-hr	LC50	0.023
Esters	: Fish (SW)		ChV	0.056
Esters	: Mysid (SW)	14	ChV	0.000318
Esters	: Earthworm	14-day	LC50	190.265 *
		=======	=====	========
Neutral Organic SAR	: Fish	96-hr	LC50	0.046
(Baseline Toxicity)	: Daphnid	48-hr	LC50	0.038
(: Green Algae	96-hr	EC50	0.142
	: Fish		ChV	0.007
	: Daphnid		ChV	0.011
	: Green Algae		ChV	0.088

Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10X, typically no effects at saturation (NES) are reported.

Class Specific LogKow Cut-Offs

If the log Kow of the chemical is greater than the endpoint specific cut-offs presented below, then no effects at saturation are expected for those endpoints.

Esters:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)

Maximum LogKow: 6.0 (Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)

Baseline Toxicity SAR Limitations:

Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50) Maximum LogKow: 6.4 (Green Algae EC50) Maximum LogKow: 8.0 (ChV)

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```

 HENRYWIN (v3.20) Program Results:

Bond Est: 7.39E-007 atm-m3/mole (7.49E-002 Pa-m3/mole) Group Est: 6.43E-008 atm-m3/mole (6.52E-003 Pa-m3/mole)

SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

MOL FOR: C20 H26 O4 MOL WT : 330.43

----- HENRYWIN v3.21 Results ------

Experimental Database Structure Match: : DICYCLOHEXYL PHTHALATE Name

CAS Num 000084-61-7

Exp HLC : 1.00E-07 atm-m3/mole (0.0101 Pa-m3/mole)
Temper : 25 deg C
Exp Ref : VP/WSOL

	<u> </u>	L	
CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN HYDROGEN FRAGMENT FRAGMENT FRAGMENT FRAGMENT FRAGMENT	22 Hydrogen to Carbon (aliphatic) Bonds 4 Hydrogen to Carbon (aromatic) Bonds 12 C-C 2 C-O 6 Car-Car 2 Car-CO 2 CO-O		-2.6329 -0.6172 1.3956 2.1709 1.5828 2.4775 0.1429
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	TOTAL	4.520

HENRYS LAW CONSTANT at 25 deg C = 7.39E-007 atm-m3/mole = 3.02E-005 unitless = 7.49E-002 Pa-m3/mole

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	10 CH2 (C)(C) 2 CH (C)(C)(0) 4 Car-H (Car)(Car) 2 Car (Car)(Car)(C0) 2 CO (0)(Car) 2 0 (C)(CO)		-1.50 0.24 0.44 -1.68 9.14 -1.06
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	5.58

HENRYS LAW CONSTANT at 25 deg C = 6.43E-008 atm-m3/mole = 2.63E-006 unitless = 6.52E-003 Pa-m3/mole

For Henry LC Comparison Purposes:

Exper Database: 1.00E-07 atm-m3/mole (1.01E-002 Pa-m3/mole)
User-Entered Henry LC: 9.446E-008 atm-m3/mole (9.571E-003 Pa-m3/mole) Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:
HLC: 2.553E-007 atm-m3/mole (2.587E-002 Pa-m3/mole)
VP: 8.69E-007 mm Hg (source: User-Entered)

WS: 1.48 mg/L (source: User-Entered)

Log Octanol-Air (KOAWIN v1.10) Results: _____

December 2024 3704 Log Koa: 10.233 SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43 ------ KOAWIN imes 1.10 Results ------Log Koa (octanol/air) estimate: 10.233 Koa (octanol/air) estimate: 1.711e+010 3714 Using: Log Kow: 4.82 (user entered)
HenryLC: 9.45e-008 atm-m3/mole (user entered)
Log Kaw: -5.413 (air/water part.coef.) LogKow : ---- (exp database) LogKow : 6.20 (KowWin estimate) Henry LC: 1e-007 atm-m3/mole (exp database) Henry LC: 7.39e-007 atm-m3/mole (HenryWin bond estimate) 3723 3724 Log Koa (octanol/air) estimate: 10.720 (from KowWin/HenryWin) 3726 $37\overline{27}$ $37\overline{28}$ BIOWIN (v4.10) Program Results: **2**9 _____ SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43 3732 ----- BIOWIN v4.10 Results Biowin1 (Linear Model Prediction) : Biodegrades Fast Biowin2 (Non-Linear Model Prediction): Biodegrades Fast Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months Biowin4 (Primary Biodegradation Timeframe): Days Biowin5 (MITI Linear Model Prediction): Biodegrades Fast Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast Ready Biodegradability Prediction: NO TYPE | NUM | Biowin1 FRAGMENT DESCRIPTION | COEFF | VALUE

Frag | 2 | Ester [-C(=0)-O-C] | 0.1742 | 0.3484

Molwt | * | Molecular Weight Parameter | -0.1573

Const | * | Equation Constant | 0.7475 3749́ 3752 RESULT | Biowin1 (Linear Biodeg Probability) | 0.9386 ______+__+__+__+ TYPE | NUM | Biowin2 FRAGMENT DESCRIPTION | COEFF | VALUE Frag | 2 | Ester [-C(=0)-O-C] | 4.0795 | 8.1590 MolWt| * | Molecular Weight Parameter | | -4.6921 RESULT | Biowin2 (Non-Linear Biodeg Probability) | 0.9985 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast _____ TYPE | NUM | Biowin3 FRAGMENT DESCRIPTION | COEFF | VALUE

3836

		December 2024				
Frag MolWt Const	: .	Ester [-C(=0)-0-C] 0.1402 0.2804 Molecular Weight Parameter -0.7307 Equation Constant 3.1997				
RESU	-	Biowin3 (Survey Model - Ultimate Biodeg) 		2.7494		
		TT				
TYPE	NUM Biowin4 FRAGMENT DESCRIPTION COEFF		VALUE			
Frag MolWt Const		* Molecular Weight Parameter -0.4767 * Equation Constant 3.8477				
RESU		+============+++++++++++++++++++++++++		3.8289		
Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks (Primary & Ultimate) 2.00 -> months 1.00 -> longer			•			
TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION COEFF		VALUE		
Frag Frag Frag Frag MolWt	Frag 4 Aromatic-H 0.0004 0.0010 Frag 10 -CH2- [cyclic] 0.0141 0.141 Frag 2 -CH - [cyclic] 0.0079 0.015 MolWt * Molecular Weight Parameter -0.521		0.4638 0.0016 0.1411 0.0158 -0.5211 0.5544			
RESU	_			0.6556		
TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE		
Frag Frag Frag Frag MolWt	Frag 4 Aromatic-H 0.0342 0.1368 Frag 10 -CH2- [cyclic] 0.1206 1.2058 Frag 2 -CH - [cyclic] 0.0294 0.0589			0.1368 1.2058 0.0589		
RESULT Biowin6 (MITI Non-Linear Biodeg Probability) 0.6257						
		· '	'	•		

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable A Probability Less Than 0.5 indicates --> NOT Readily Degradable

TYPE NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag 2 Frag 4 Frag 10 Frag 2 Const *	Ester [-C(=0)-0-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Equation Constant	0.1719 -0.0954 -0.1200 0.0395	0.3437 -0.3817 -1.2001 0.0789 0.8361
RESULT		+======= -===========================	-0.3232

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey

December 2024

```
model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for
degradation in the OECD301C test only; using data from the Chemicals
Evaluation and Research Institute Japan (CERIJ) database.
```

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3856 3857

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3863 3864

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3868 3869 3870

3879

3880 3881

3883

3884 3885 3886

3888

3889 3890

3891

3892

3893

3894

3895

3896 3897

3898 3899

3900

3901

3902

```
BioHCwin (v1.01) Program Results:
SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
      : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
               NO Estimate Possible ... Structure NOT a Hydrocarbon
    (Contains atoms other than C, H or S (-S-))
AEROWIN Program (v1.00) Results:
 Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
  Vapor pressure (liquid/subcooled): 0.000295 Pa (2.21E-006 mm Hg)
  Log Koa (Koawin est ): 10.233
   Kp (particle/gas partition coef. (m3/ug)):
   Mackay model : 0.0102
Octanol/air (Koa) model: 0.0042
Fraction sorbed to airborne particulates (phi):
       Junge-Pankow model : 0.269
       Mackay model
                                  0.449
       Octanol/air (Koa) model: 0.251
AOP Program (v1.92) Results:
SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
         ----- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) ------
Hydrogen Abstraction = 23.5226 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec **Addition to Aromatic Rings = 0.7492 E-12 cm3/molecule-sec
                           = 0.0000 E-12 cm3/molecule-sec
Addition to Fused Rings
   OVERALL OH Rate Constant = 24.2718 E-12 cm3/molecule-sec
   HALF-LIFE =
                    0.441 Days (12-hr day; 1.5E6 OH/cm3)
   HALF-LIFE = 5.288 Hrs
..... ** Designates Estimation(s) Using ASSUMED Value(s)
----- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) ------
                ****** NO OZONE REACTION ESTIMATION ******
                (ONLY Olefins and Acetylenes are Estimated)
Experimental Database: NO Structure Matches
Fraction sorbed to airborne particulates (phi):
  0.359 (Junge-Pankow, Mackay avg)
  0.251 (Koa method)
     Note: the sorbed fraction may be resistant to atmospheric oxidation
```

```
3906
3907
3908
      KOCWIN Program (v2.00) Results:
3909
3910
      SMILES: 0=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCCC3)C3)c2
3911
            : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
3912
      MOL FOR: C20 H26 O4
3913
      MOL WT : 330.43
3914
3915
              ------ KOCWIN v2.01 Results ----------
        Koc Estimate from MCI:
3918
               First Order Molecular Connectivity Index .....: 11.737
               Non-Corrected Log Koc (0.5213 MCI + 0.60) ...... : 6.7184
               Fragment Correction(s):
                            Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -2.5939
3922
               Corrected Log Koc ..... 4.1245
                               Estimated Koc: 1.332e+004 L/kg <=======
3925
3926
        Koc Estimate from Log Kow:
               Log Kow (User entered
               Non-Corrected Log Koc (0.55313 logKow + 0.9251) ....:
                                                                        3.5912
               Fragment Correction(s):
                            Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -0.1312
               Corrected Log Koc .....: 3.4600
                               Estimated Koc: 2884 L/kg <=======
3939
      HYDROWIN Program (v2.00) Results:
3940
3941
      SMILES: 0=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCCC3)C3)c2
            : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
3942
3943
      MOL FOR: C20 H26 O4
3944
      MOL WT : 330.43
3945
                 ------ HYDROWIN v2.00 Results -------
3946
3947
3948
      NOTE: Fragment(s) on this compound are NOT available from the fragment
3949
           library. Substitute(s) have been used!!! Substitute R1, R2, R3,
3950
          or R4 fragments are marked with double astericks "**"
3951
3952
      ESTER: R1-C(=0)-0-R2
                                           ** R1: -Phenyl
3953
       R2: -cyclohexyl
NOTE: Ortho-position fragments(s) on Phenyl ring(s) are NOT CONSIDERED!!
3955
       Kb hydrolysis at atom # 2: 9.417E-003 L/mol-sec
3956
3957
      ESTER: R1-C(=0)-0-R2
                                              R1: -Phenyl
3958
                                              R2: -cyclohexyl
3959
       Kb hydrolysis at atom # 15: 9.417E-003 L/mol-sec
3960
       Total Kb for pH > 8 at 25 deg C : 1.883E-002 L/mol-sec Kb Half-Life at pH 8: 1.166 years Kb Half-Life at pH 7: 11.662 years
3961
3962
3963
3964
3965
3966
3967
3968
      BCFBAF Program (v3.01) Results:
3969
3970
      SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
```

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```
CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43
3971
3972
397<del>3</del>
                          ------ BCFBAF v3.01 -----
3974
3975
        Summary Results:
          Log BCF (regression-based estimate): 2.85 (BCF = 703 L/kg wet-wt)
Biotransformation Half-Life (days): 0.159 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 1.83 (BAF = 67.1 L/kg wet-wt)
3976
3977
3978
3979
3980
        Log Kow (experimental): not available from database
3981
3982
        Log Kow used by BCF estimates: 4.82 (user entered)
3983
        Equation Used to Make BCF estimate:
3984
            Log BCF = 0.6598 \log Kow - 0.333 + Correction
3985
3986
                Correction(s):
                                                         Value
3987
                 No Applicable Correction Factors
3988
3989
            Estimated Log BCF = 2.847 (BCF = 703.5 L/kg wet-wt)
3990
3991
        _____
3992
        Whole Body Primary Biotransformation Rate Estimate for Fish:
3993
        3994
3995
         TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
        3996
         3997
3998
3999
4000
4001
4002
4003
4004
4005
           4006
                                                                                          | -0.7986
4007
                                                                                               0.159
4008
4009
4010
4011
        Biotransformation Rate Constant:
         kM (Rate Constant): 4.359 /day (10 gram fish)
kM (Rate Constant): 2.451 /day (100 gram fish)
kM (Rate Constant): 1.378 /day (1 kg fish)
kM (Rate Constant): 0.7752 /day (10 kg fish)
4012
4013
4014
4015
4016
4017
        Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
           Estimated Log BCF (upper trophic) = 1.827 (BCF = 67.13 L/kg wet-wt) Estimated Log BAF (upper trophic) = 1.827 (BAF = 67.13 L/kg wet-wt) Estimated Log BCF (mid trophic) = 1.959 (BCF = 90.99 L/kg wet-wt) Estimated Log BAF (mid trophic) = 1.962 (BAF = 91.63 L/kg wet-wt) Estimated Log BCF (lower trophic) = 1.999 (BCF = 99.71 L/kg wet-wt) Estimated Log BAF (lower trophic) = 2.031 (BAF = 107.3 L/kg wet-wt)
4018
4019
4020
4021
4022
4023
4024
4025
        Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
            Estimated Log BCF (upper trophic) = 3.758 (BCF = 5725 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 4.731 (BAF = 5.377e+004 L/kg wet-wt)
4026
4027
4028
4029
4030
4031
4032
4033
                                           Volatilization From Water
4034
                                           _____
4035
4036
        Chemical Name: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
```

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```
Molecular Weight : 330.43 g/mole
Water Solubility : 1.48 ppm
Vapor Pressure : 8.69E-007 mm Hg
Henry's Law Constant: 9.45E-008 atm-m3/mole (entered by user)
4038
4039
4040
4041
4042
4043
                                                                               RIVER
                                                                                                                       LAKE
4044
               Water Depth (meters): 1
Wind Velocity (m/sec): 5
4045
                                                                                                                    1
4046
                                                                                                                      0.5
4047
               Current Velocity (m/sec):
                                                                             1
                                                                                                                      0.05
4048
4049
                            HALF-LIFE (hours) : 1.127E+004
HALF-LIFE (days ) : 469.5
HALF-LIFE (years) : 1.286
                                                                                                              1.231E+005
5129
4050
4051
                                                                                                                     14.04
4052
4053
4054
               STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
4055
                                       -----
4056
                      (using 10000 hr Bio P,A,S)
4057
               PROPERTIES OF: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
4058
4059
               Molecular weight (g/mol)
Aqueous solubility (mg/l)
4060
                                                                                                                                           1.48
4061
                                                                                                                                          0.000115857
               Vapour pressure (Pa)
4062
                                                   (atm)
                                                                                                                                          1.14342E-009
                                                                                                                                          8.69E-007
4063
                                                   (mm Hg)
4064
               Henry 's law constant (Atm-m3/mol)
                                                                                                                                          9.446E-008
4065
               Air-water partition coefficient
                                                                                                                                          3.86313E-006
4066
               Octanol-water partition coefficient (Kow)
                                                                                                                                          66069.4
4067
                                                                                                                                          4.82
               Biomass to water partition coefficient 
Temperature [deg C]
4068
                                                                                                                                          13214.7
4069
                                                                                                                                          25
               Biodeg rate constants (h\^-1), half life in biomass (h) and in 2000 mg/L MLSS (h):

-\text{Primary tank}
0.00
9635.43
10000.00
4070
4071
                                                                                                                                          10000.00
4072
                                      -Aeration tank
                                                                                    0.00
                                                                                                           9635.43
4073
                                                                                                          9635.43
                                                                                    0.00
                                                                                                                                          10000.00
                                     -Settling tank
4074
4075
                 STP Overall Chemical Mass Balance:
4076
4077
4078
                                                                               g/h
                                                                                                                        mol/h
                                                                                                                                                          percent
4079
               Influent
                                                                                                                      3.0E-002
                                                                              1.00E+001
                                                                                                                                                          100.00
4080
                                                                                                                                                  43.54
27.02
               ### 1.35E+000 ### 1.3E-002 ### 2.70E+000 ### 8.2E-003 ### 8.2E-003 ### 8.2E-008 ###
4081
4082
4083
                                                                                                                                                       0.00
4084
                                                                                                                                                           0.00
4085
                                                                                                                                                            0.00
4086
               Primary biodegradation
Settling biodegradation
Aeration biodegradation
4087
                                                                             1.32E-002
3.53E-003
                                                                                                                     4.0E-005
                                                                                                                                                           0.13
4088
                                                                                                                      1.1E-005
                                                                                                                                                            0.04
                                                                             4.65E-002
4089
                                                                                                                      1.4E-004
                                                                                                                                                           0.47
4090
4091
               Final water effluent
                                                                              2.88E+000
                                                                                                                     8.7E-003
                                                                                                                                                          28.81
4092
4093
                                                                            7.12E+000
6.32E-002
               Total removal
                                                                                                                    2.2E-002
                                                                                                                                                         71.19
               Total biodegradation
4094
                                                                                                                      1.9E-004
                                                                                                                                                            0.63
4095
4096
4097
4098
               STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
4099
                               ______
                       (using Biowin/EPA draft method)
4100
               PROPERTIES OF: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
4101
4102
4103
                                                                                                                                           330.43
               Molecular weight (g/mol)
```

1.48

4104

Aqueous solubility (mg/l)

```
4105
       Vapour pressure (Pa)
                                                                    0.000115857
4106
                          (atm)
                                                                     1.14342E-009
4107
                         (mm Hq)
                                                                     8.69E-007
4108
       Henry 's law constant (Atm-m3/mol)
                                                                    9.446E-008
4109
       Air-water partition coefficient
                                                                     3.86313E-006
                                                                     66069.4
4110
       Octanol-water partition coefficient (Kow)
                                                                     4.82
4111
       Log Kow
4112
       Biomass to water partition coefficient
                                                                     13214.7
4113
       Temperature [deg C]
                                                                     25
4114
       Biodeg rate constants (h^-1), half life in biomass (h) and in 2000 mg/L MLSS (h):
                                    0.01
4115
                                                                       100.00
                  -Primary tank
                                                       96.35
4116
                   -Aeration tank
                                          0.07
                                                        9.64
                                                                        10.00
4117
                                                        9.64
                                                                        10.00
                   -Settling tank
                                          0.07
4118
4119
         STP Overall Chemical Mass Balance:
4120
4121
                                        g/h
                                                           mol/h
                                                                            percent
4122
4123
       Influent
                                       1.00E+001
                                                          3.0E-002
                                                                            100.00
4124
4125
4126
4127
4128
       Primary sludge
Waste sludge
                                       3.85E+000
                                                          1.2E-002
                                                                            38.51
                                       2.37E-001
                                                          7.2E-004
                                                                             2.37
                                       1.25E-005
                                                                             0.00
       Primary volatilization
                                                          3.8E-008
       Settling volatilization
                                       3.02E-006
                                                          9.1E-009
                                                                             0.00
4129
       Aeration off gas
                                       7.61E-006
                                                          2.3E-008
                                                                             0.00
4130
4131
                                       1.17E+000
                                                          3.5E-003
                                                                            11.68
       Primary biodegradation
4132
                                                                             3.10
       Settling biodegradation
                                       3.10E-001
                                                          9.4E-004
4133
4134
4135
       Aeration biodegradation
                                       4.18E+000
                                                          1.3E-002
                                                                            41.81
       Final water effluent
                                       2.53E-001
                                                          7.7E-004
                                                                             2.53
4136
4137
       Total removal
                                       9.75E+000
                                                          2.9E-002
                                                                            97.47
4138
                                       5.66E+000
       Total biodegradation
                                                          1.7E-002
                                                                            56.59
4139
         (** Total removal recommended maximum is 95 percent)
4140
4141
4142
4143
       Level III Fugacity Model (Full-Output): MCI Method
4144
          Chem Name : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
         Molecular Wt: 330.43
Henry's LC: 9.45e-008 atm-m3/mole (user-entered)
4145
4146
         Henry's LC : 9.45e-008 atm-m3/mole (user-ent Vapor Press : 8.69e-007 mm Hg (user-entered)
4147
4148
          Liquid VP : 2.21e-006 mm Hg (super-cooled)
4149
                      : 66 deg C (user-entered)
          Melting Pt
4150
                       : 4.82 (user-entered)
          Log Kow
4151
4152
4153
          Soil Koc
                       : 1.33e+004 (KOCWIN MCI method)
                                    Half-Life
                    Mass Amount
                                                   Emissions
4154
                     (percent)
                                        (hr)
                                                    (kg/hr)
4155
                      9.98e-005
                                        10.6
           Air
                                                      O
4156
                      0.0477
                                        900
                                                      0
           Water
                                        1.8e+003
4157
           Soil
                      99.9
                                                      1000
4158
                                        8.1e+003
           Sediment 0.0367
4159
4160
                      Fugacity
                                   Reaction
                                                 Advection
                                                              Reaction
                                                                           Advection
4161
                       (atm)
                                   (kg/hr)
                                                  (kg/hr)
                                                              (percent)
                                                                           (percent)
                                                  0.0259
                      1.36e-015
                                    0.17
                                                                            0.00259
4162
           Air
                                                               0.017
                      1.73e-015
4163
           Water
                                    0.952
                                                 1.24
                                                               0.0952
                                                                            0.124
4164
           Soil
                      1.29e-013
                                    998
                                                  0
                                                               99.8
                                                                            0
4165
           Sediment 2.12e-015
                                                 0.019
                                                                            0.0019
                                    0.0814
                                                               0.00814
4166
4167
           Persistence Time: 2.59e+003 hr
4168
           Reaction Time:
                               2.6e+003 hr
4169
           Advection Time:
                               2.02e+006 hr
4170
                              99.9
           Percent Reacted:
4171
           Percent Advected: 0.128
```

```
4172
4173
           Water Compartment Percents:
4174
4175
                                     Half-Life
                    Mass Amount
                                                    Emissions
4176
                     (percent)
                                        (hr)
                                                     (kg/hr)
4177
           Air
                      9.98e-005
                                        10.6
                                                       Ŏ
4178
                      0.0477
                                        900
                                                       0
           Water
4179
                         (0.0466)
             water
4180
                         (0.000154)
             biota
4181
             suspended sediment (0.000931)
4182
4183
                      99.9
                                        1.8e+003
           Soil
                                                       1000
           Sediment 0.0367
                                        8.1e+003
                                                       0
4184
           Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin): Air: 10.58
4185
4186
4187
                          900
              Water:
4188
              soil:
                          1800
4189
              Sediment: 8100
4190
                 Biowin estimate: 2.749 (weeks-months)
4191
4192
           Advection Times (hr):
4193
                         100
              Air:
4194
              water:
                          1000
4195
              Sediment: 5e+004
4196
4197
4198
       Level III Fugacity Model (Full-Output): EQC Default
4199
          Chem Name : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester Molecular Wt: 330.43
4200
4201
          Henry's LC : 9.45e-008 atm-m3/mole (user-entered) 
Vapor Press : 8.69e-007 mm Hg (user-entered)
4202
4203
          Liquid VP
4204
                        : 2.21e-006 mm Hg
                                             (super-cooled)
4205
          Melting Pt
                       : 66 deg C (user-entered)
4206
          Log Kow
                       : 4.82 (user-entered)
4207
                        : 2.71e+004
                                     (EQC Model Default)
          Soil Koc
4208
4209
                                     Half-Life
                    Mass Amount
                                                    Emissions
4210
                                        (hr)
                     (percent)
                                                     (kg/hr)
4211
                      4.91e-005
                                        10.6
                                                       0
           Air
                      0.0251
                                        900
                                                       0
           Water
4213
                      99.9
                                        1.8e+003
                                                       1000
           Soil
4214
                      0.0387
                                        8.1e+003
                                                       0
           Sediment
4215
4216
                      Fugacity
                                    Reaction
                                                 Advection
                                                               Reaction
                                                                             Advection
4217
                       (atm)
                                    (kg/hr)
                                                   (kg/hr)
                                                               (percent)
                                                                             (percent)
4218
                      6.7e-016
                                     0.0836
                                                   0.0128
                                                                0.00836
                                                                              0.00128
           Air
4219
                                                  0.652
                      8.92e-016
                                     0.502
                                                                0.0502
                                                                              0.0652
           Water
4220
                                     999
                                                                99.9
           Soil
                      6.33e-014
                                                                              0
           Sediment
                     1.1e-015
                                     0.0859
                                                   0.0201
                                                                0.00859
                                                                              0.00201
           Persistence Time: 2.6e+003 hr
           Reaction Time:
                               2.6e+003 hr
                               3.79e+006 hr
           Advection Time:
4226
           Percent Reacted: 99.9
\frac{4227}{4228}
           Percent Advected: 0.0685
4229
           Water Compartment Percents:
4230
                                     Half-Life
                                                    Emissions
                    Mass Amount
                                                     (kg/hr)
                     (percent)
                                        (hr)
                                        10.6
           Air
                      4.91e-005
                                                       0
                      0.0251
                                        900
                                                       0
           Water
                         (0.0241)
             water
4236
             biota
                         (7.95e-005)
             suspended sediment (0.000977)
                                        1.8e+003
4238
                      99.9
                                                       1000
```

Soil

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```
4239
              Sediment 0.0387
                                                    8.1e+003
4240
4\bar{2}41
              Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin): Air: 10.58
4242
4243
                                 900
                  Water:
4244
                  Soil:
                                 1800
4245
                  Sediment: 8100
4246
                      Biowin estimate: 2.749 (weeks-months)
4247
4248
              Advection Times (hr):
                             100
4249
                  Air:
4\overline{250}
                                 1000
                   Water:
4251
                  Sediment: 5e+004
4252
                  A.8.4 Release to Air, Water, and Soil
4253
          Run Date: 2024-06-21
4254
4255
4256
4257
          CAS Number: 000084-61-7
          SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
         CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43
4\overline{2}58
4259
4260
               ----- EPI SUMMARY (v4.11)
4261
4262
           Physical Property Inputs:
               Log Kow (octanol-water): 4.82
Boiling Point (deg C): 225.00
Melting Point (deg C): 66.00
Vapor Pressure (mm Hg): 8.69E-007
Water Solubility (mg/L): 1.48
Henry LC (atm-m3/mole): 9.446E-008
4263
                Log Kow (octanol-water):
4264
4265
4266
4267
4268
4269
4270
          KOWWIN Program (v1.68) Results:
4271
          _____
4272
                                    Log Kow(version 1.69 estimate): 6.20
4274
4275
4276
         SMILES: O=C(OC(CCC1)C1)c(c(cc2)C(=0)OC(CCC3)C3)c2 CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4
4278
          MOL WT : 330.43
4279
4280
           TYPE | NUM | LOGKOW FRAGMENT DESCRIPTION | COEFF | VALUE
4281

      Frag
      10
      -CH2- [aliphatic carbon]
      0.4911
      4.9110

      Frag
      2
      -CH [aliphatic carbon]
      0.3614
      0.7228

      Frag
      6
      Aromatic Carbon
      0.2940
      1.7640

      Frag
      2
      -C(=0)0 [ester, aromatic attach]
      -0.7121
      -1.4242

      Const
      Equation Constant
      0.2290

4283
4284
4285
4286
4287
                                                                                             Log Kow = 6.2026
4288
4290
          MPBPVP (v1.43) Program Results:
4293
          _____
4294
          Experimental Database Structure Match:
4\overline{2}95
            Name : DICYCLOHEXYL PHTHALATE CAS Num : 000084-61-7
4\overline{2}96
            Exp MP (deg C): 66
Exp BP (deg C): 224 @ 4 mm Hg
4298
4299
                                    8.69E-07 (extrapolated)
             Exp VP (mm Hg):
4300
                       (Pa ):
                                    1.16E-004
4301
             Exp VP (deg C):
                                    25
```

4302

4303

Exp VP ref : WERNER, AC (1952)

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```
4304
                  SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
                 CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT: 330.43
4305
4306
4307
4308
                   ----- SUMMARY MPBPWIN v1.44 ------
4309
4310
                  Boiling Point: 394.85 deg C (Adapted Stein and Brown Method)
4311
4312
                 Melting Point: 50.36 deg C (Adapted Joback Method)
Melting Point: 116.89 deg C (Gold and Ogle Method)
Mean Melt Pt: 83.63 deg C (Joback; Gold,Ogle Methods)
Selected MP: 61.45 deg C (Weighted Value)
4313
4314
4315
4316
4317
                  Vapor Pressure Estimations (25 deg C):
(Using BP: 225.00 deg C (user entered))
(Using MP: 66.00 deg C (user entered))
4318
4319
4320
4321
4322
4323
4324
                            VP: 0.0445 mm Hg (Antoine Method)
                                 : 5.93 Pa (Antoine Method)
                            VP: 0.0392 mm Hg (Modified Grain Method)
    : 5.22 Pa (Modified Grain Method)
                       VP: 0.0632 mm Hg (Mackay Method)
: 8.43 Pa (Mackay Method)
Selected VP: 0.0392 mm Hg (Modified Grain Method)
: 5.22 Pa (Modified Grain Method)
4325
4326
4327
43\overline{28}
4329
                       Subcooled liquid VP: 2.21E-006 mm Hg (25 deg C, user-entered VP) : 0.000295 Pa (25 deg C, user-entered VP)
4330
4331
4332
4333
                    TYPE | NUM | BOIL DESCRIPTION | COEFF | VALUE
4334
                    4335
4336
4337
4338
4339
4340
4341
4342
                  RESULT-uncorr | BOILING POINT in deg Kelvin | 804.24
RESULT- corr | BOILING POINT in deg Kelvin | 668.01
BOILING POINT in deg C | 394.85
4343
4344
4345
4346
4347
4348
                  -----+----+-----
4349
                 TYPE | NUM | MELT DESCRIPTION | COEFF | VALUE
                  Group | 10 | -CH2- (ring) | 7.75 | 77.50 | 76.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.50 | 77.
4350
4351
4352
4353
4354
4355
4356
4357
4358
                  _____+__+__+
                  RESULT | MELTING POINT in deg Kelvin | 323.52
4359
4360
                                                 | MELTING POINT in deg C | 50.36
4361
4362
4363
```

Water Sol from Kow (WSKOW v1.42) Results: _____

 Water Sol: 1.48 mg/L

Experimental Water Solubility Database Match:

```
December 2024
           Name : DICYCLOHEXYL PHTHALATE
CAS Num : 000084-61-7
Exp WSol : 4 mg/L (24 deg C)
Exp Ref : YALKOWSKY,SH & DANNENFELSER,RM (1992)
4371
4372
4373
4374
4375
4376
        SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
4377
        CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
        MOL FOR: C20 H26 O4 MOL WT : 330.43
4378
4379
4380
         ------ WSKOW v1.43 Results ------
        Log Kow (estimated): 6.20
Log Kow (experimental): not available from database
4381
4382
4383
        Log Kow used by Water solubility estimates: 4.82 (user entered)
4385
        Equation Used to Make Water Sol estimate:
4386
            Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction
4387
4388
                Melting Pt (Tm) = 66.00 \text{ deg C (Use } Tm = 25 \text{ for all liquids})
4389
4390
                Correction(s):
                                            Value
4391
4392
                 No Applicable Correction Factors
4393
            Log Water Solubility (in moles/L): -5.349 Water Solubility at 25 deg C (mg/L): 1.48
4394
4395
4396
4397
4398
4399
        WATERNT Program (v1.01) Results:
4400
        4401
4402
                            Water Sol (v1.01 est): 2.4027 \text{ mg/L}
4403
4404
        Experimental Water Solubility Database Match:
           Name : DICYCLOHEXYL PHTHALATE
CAS Num : 000084-61-7
Exp WSol : 4 mg/L (24 deg C)
4405
4406
4407
4408
           Exp Ref : YALKOWSKY, SH & DANNENFELSER, RM (1992)
4409
        SMILES : 0=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCCC3)C3)c2 CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4
4410
4411
4412
4413
        MOL WT : 330.43
4414
         ------
4415
         TYPE | NUM | WATER SOLUBILITY FRAGMENT DESCRIPTION | COEFF | VALUE
        Frag | 2 | -CH [aliphatic carbon]
Frag | 4 | Aromatic Carbon (C-H type)
Frag | 2 | -C(=0)0 [ester, aromatic attach]
Frag | 2 | Aromatic Carbon (C-substituent type)
Frag | 10 | -CH2- [aliphatic carbon, cyclic]
Const | Equation Constant
4416
                                                                                4417
4418
4419
4420
4421
4422
                                                                                              0.2492
4423
                                            Log Water Sol (moles/L) at 25 dec C = -5.1384
                                             water Solubility (mg/L) at 25 dec C = 2.4027
4428
4429
        ECOSAR Program (v1.11) Results:
4430
        _____
4431
        ECOSAR Version 1.11 Results Page
4432
```

SMILES: 0=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCCC3)C3)c2
CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

4435 CAS Num: 4436 ChemID1:

MOL FOR: C20 H26 O4

```
MOL WT: 330.43
Log Kow: 6.203
Log Kow:
Log Kow:
4438
         Log Kow: (PhysProp DB exp value - for comparison only)
Melt Pt: 66.00 (deg C, User Entered for Wat Sol estimate)
Wat Sol: 0.06964
Wat Sol: 1.48
Wat Sol: 4 (mg/L, EpiSuite WSKowwin v1.43 Estimate)
Wag/L, PhysProp DB
4439
4440
4441
4442
4443
4444
4445
4446
4447
4448
4449
4450
           Values used to Generate ECOSAR Profile
          Log Kow: 6.203 (EpiSuite Kowwin v1.68 Estimate) Wat Sol: 1.48 (mg/L, User Entered)
4451
4452
4453
4454
4455
4456
4457
4458
           ECOSAR v1.11 Class-specific Estimations
4459
4460
           Esters
4461
                                                                                                                       Predicted
          ECOSAR Class
                                                  Organism Duration End Pt mg/L (ppm)
4462
4463
          Esters : Fish 96-hr LC50 0.155
Esters : Daphnid 48-hr LC50 0.206
Esters : Green Algae 96-hr EC50 0.045
Esters : Daphnid ChV 0.005
Esters : Green Algae ChV 0.042
Esters : Green Algae ChV 0.045
Esters : Fish (SW) 96-hr LC50 0.183
Esters : Mysid 96-hr LC50 0.023
Esters : Fish (SW) ChV 0.056
Esters : Mysid (SW) ChV 0.00518
Esters : Earthworm 14-day LC50 190.265 *
4464
4465
4466
4467
4468
4469
4470
4471
4472
4473
4474
          Neutral Organic SAR : Fish 96-hr LC50 0.046
(Baseline Toxicity) : Daphnid 48-hr LC50 0.038
: Green Algae 96-hr EC50 0.142
: Fish ChV 0.007
: Daphnid ChV 0.011
: Green Algae ChV 0.088
4475
4476
4477
4478
4479
4480
4481
4482
4483
            Note: * = asterisk designates: Chemical may not be soluble enough to measure this predicted effect. If the effect level exceeds the water solubility by 10x, typically no effects at saturation (NES)
4484
4485
4486
                       are reported.
4488
4489
4490
           Class Specific LogKow Cut-Offs
4491
4492
4493
           If the log Kow of the chemical is greater than the endpoint specific cut-offs
           presented below, then no effects at saturation are expected for those endpoints.
4494
4495
4496
4497
4498
           Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50, Mysid LC50)
          Maximum LogKow: 6.0 (Earthworm LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
4499
4500
4501
4502
4503
           Baseline Toxicity SAR Limitations:
```

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```
Maximum LogKow: 5.0 (Fish 96-hr LC50; Daphnid LC50)
Maximum LogKow: 6.4 (Green Algae EC50)
Maximum LogKow: 8.0 (ChV)
4505
4506
```

HENRYWIN (v3.20) Program Results:

Bond Est: 7.39E-007 atm-m3/mole (7.49E-002 Pa-m3/mole) Group Est: 6.43E-008 atm-m3/mole (6.52E-003 Pa-m3/mole)

SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

MOL FOR: C20 H26 O4 MOL WT : 330.43

------ HENRYWIN v3.21 Results -----------

Experimental Database Structure Match:

Name : DICYCLOHEXYL PHTHALATE
CAS Num : 000084-61-7
Exp HLC : 1.00E-07 atm-m3/mole (0.0101 Pa-m3/mole)
Temper : 25 deg C
Exp Ref : VP/WSOL

	l		
CLASS	BOND CONTRIBUTION DESCRIPTION	COMMENT	VALUE
HYDROGEN HYDROGEN FRAGMENT FRAGMENT FRAGMENT FRAGMENT FRAGMENT	22 Hydrogen to Carbon (aliphatic) Bonds 4 Hydrogen to Carbon (aromatic) Bonds 12 C-C 2 C-O 6 Car-Car 2 Car-CO 2 CO-O		-2.6329 -0.6172 1.3956 2.1709 1.5828 2.4775 0.1429
RESULT BOND ESTIMATION METHOD for LWAPC VALUE		TOTAL	4.520

HENRYS LAW CONSTANT at 25 deg C = 7.39E-007 atm-m3/mole = 3.02E-005 unitless = 7.49E-002 Pa-m3/mole

	GROUP CONTRIBUTION DESCRIPTION	COMMENT	VALUE
	10 CH2 (C)(C) 2 CH (C)(C)(0) 4 Car-H (Car)(Car) 2 Car (Car)(Car)(C0) 2 CO (0)(Car) 2 0 (C)(CO)		-1.50 0.24 0.44 -1.68 9.14 -1.06
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL	5.58

HENRYS LAW CONSTANT at 25 deg C = 6.43E-008 atm-m3/mole = 2.63E-006 unitless = 6.52E-003 Pa-m3/mole

For Henry LC Comparison Purposes:

Exper Database: 1.00E-07 atm-m3/mole (1.01E-002 Pa-m3/mole)
User-Entered Henry LC: 9.446E-008 atm-m3/mole (9.571E-003 Pa-m3/mole) Henrys LC [via VP/WSol estimate using User-Entered or Estimated values]:

HLC: 2.553E-007 atm-m3/mole (2.587E-002 Pa-m3/mole)

8.69E-007 mm Hg (source: User-Entered)

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WS: 1.48 mg/L (source: User-Entered)

```
4572
4573
4574
4575
```

```
Log Octanol-Air (KOAWIN v1.10) Results:
         Log Koa: 10.233
```

SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4 MOL WT : 330.43

Log Koa (octanol/air) estimate: 10.233 Koa (octanol/air) estimate: 1.711e+010 Using:

Log Kow: 4.82 (user entered)

HenryLC: 9.45e-008 atm-m3/mole (user entered)

Log Kaw: -5.413 (air/water part.coef.)

LogKow : ---- (exp database) LogKow : 6.20 (KowWin estimate)

Henry LC: 1e-007 atm-m3/mole (exp database)

Henry LC: 7.39e-007 atm-m3/mole (HenryWin bond estimate)

Log Koa (octanol/air) estimate: 10.720 (from KowWin/HenryWin)

BIOWIN (v4.10) Program Results:

SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

MOL FOR: C20 H26 O4 MOL WT : 330.43

----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Biodegrades Fast): Biodegrades Fast Biowin2 (Non-Linear Model Prediction): Biowin3 (Ultimate Biodegradation Timéframe): Weeks-Months

Biowin4 (Primary Biodegradation Timeframe): Days

Biowin5 (MITI Linear Model Prediction) : Biodegrades Fast Biowin6 (MITI Non-Linear Model Prediction): Biodegrades Fast Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast Ready Biodegradability Prediction: NO

	·	_	
TYPE NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag 2 Ester [-C(=0)-O-C] Molwt * Molecular Weight Parameter Const * Equation Constant		0.1742	0.3484 -0.1573 0.7475
RESULT	 Biowin1 (Linear Biodeg Probability)	=+====================================	0.9386
		_	r=======
TYPE NUM Biowin2 FRAGMENT DESCRIPTION		COEFF	VALUE

TYPE NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag 2 MolWt *	Ester [-C(=0)-O-C] Molecular Weight Parameter	4.0795	8.1590 -4.6921
RESULT	Biowin2 (Non-Linear Biodeg Probability)	-=======	0.9985

 December 2024

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast

A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

	L 	·		L	
TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag MolWt Const	2 * *	Ester [-C(=0)-O-C] 0.1402 Molecular Weight Parameter Equation Constant			
RESU		Biowin3 (Survey Model - Ultimate Biodeg)		2.7494	
TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag MolWt Const	Molwt * Molecular Weight Parameter -0.4 Const * Equation Constant 3.8		0.4579 -0.4767 3.8477		
RESU		+=====================================		3.8289	
Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks (Primary & Ultimate) 2.00 -> months 1.00 -> longer			•		
TYPE	NUM	Biowin5 FRAGMENT DESCRIPTION	C0EFF	VALUE	
Frag 4 Aromatic-H 0.0004 Frag 10 -CH2- [cyclic] 0.0141 Frag 2 -CH - [cyclic] 0.0079		0.4638 0.0016 0.1411 0.0158 -0.5211 0.5544			
RESU	=====- JLT	Biowin5 (MITI Linear Biodeg Probability)	-======	0.6556	
	-===-	+=====================================	-=======	-======	
TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE	
Frag Frag Frag Frag MolWt	2 4 10 2 *	Ester [-C(=0)-0-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Molecular Weight Parameter	1.5833 0.0342 0.1206 0.0294	3.1665 0.1368 1.2058 0.0589 -5.7164	
RESU	RESULT Biowin6 (MITI Non-Linear Biodeg Probability) 0.6257				

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable A Probability Less Than 0.5 indicates --> NOT Readily Degradable

тт		T	Г
TYPE NUM B	iowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag 4 Aromat Frag 10 -CH2- Frag 2 -CH -	[-C(=0)-0-C] ic-H [cyclic] [cyclic] on Constant	0.1719 -0.0954 -0.1200 0.0395	0.3437 -0.3817 -1.2001 0.0789 0.8361
RESULT Biowi	n7 (Anaerobic Linear Biodeg Prob)	+======= =========================	-0.3232

```
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4706
          A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
4707
          A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast
47Ŏ8
4709
         Ready Biodegradability Prediction: (YES or NO)
4710
          Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not
4711
4712
4713
4714
          satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals
4715
4716
4717
4718
4719
          Evaluation and Research Institute Japan (CERIJ) database.
4720
4721
47\bar{2}\bar{3}
4724
         BioHCwin (v1.01) Program Results:
4725
4726
4727
4728
4729
         SMILES: O=C(OC(CCCC1)C1)c(c(ccc2)C(=0)OC(CCC3)C3)c2
CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT: 330.43
4730
                     ----- BioHCwin v1.01 Results ------
4731
4732
           NO Estimate Possible ... Structure NOT a Hydrocarbon
4733
              (Contains atoms other than C, H or S (-S-))
4734
4735
4736
4737
         AEROWIN Program (v1.00) Results:
4738
4739
          Sorption to aerosols (25 Dec C)[AEROWIN v1.00]:
           Vapor pressure (liquid/subcooled): 0.000295 Pa (2.21E-006 mm Hg)
4740
4741
            Log Koa (Koawin est ): 10.233
4742
             Kp (particle/gas partition coef. (m3/ug)):
4743
                                                   0.0102
                  Mackay model
4744
                  Octanol/air (Koa) model: 0.0042
4745
             Fraction sorbed to airborne particulates (phi):
4746
                  Junge-Pankow model : 0.269
4747
                  Mackay model
                                                    0.449
4748
                  Octanol/air (Koa) model: 0.251
4749
4750
4751
         AOP Program (v1.92) Results:
4752
4753
         SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
4754
         CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
4755
         MOL FOR: C20 H26 O4 MOL WT : 330.43
4756
4757
                  ----- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C)
         Hydrogen Abstraction = 23.5226 E-12 cm3/molecule-sec Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
4758
4759
4760
         Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
4761
         Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
4762
         **Addition to Aromatic Rings = 0.7492 E-12 cm3/molecule-sec
4763
         Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec
4764
4765
             OVERALL OH Rate Constant = 24.2718 E-12 cm3/molecule-sec
4766
                                  0.441 Days (12-hr day; 1.5E6 OH/cm3)
             HALF-LIFE =
                             0.441 Day:
5.288 Hrs
```

***** NO OZONE REACTION ESTIMATION ***** (ONLY Olefins and Acetylenes are Estimated)

..... ** Designates Estimation(s) Using ASSUMED Value(s) ----- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----

4767

4768

4769 4770

4771 4772 HALF-LIFE =

```
4773
4774
      Experimental Database: NO Structure Matches
4775
      Fraction sorbed to airborne particulates (phi): 0.359 (Junge-Pankow, Mackay avg)
4776
4777
        0.251 (Koa method)
4778
            Note: the sorbed fraction may be resistant to atmospheric oxidation
4779
4780
4781
4782
4783
      KOCWIN Program (v2.00) Results:
4785
      SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
      CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester MOL FOR: C20 H26 O4
4786
4787
4788
      MOL WT : 330.43
       ------ KOCWIN v2.01 Results -----
4789
4790
4791
        Koc Estimate from MCI:
4792
4793
                First Order Molecular Connectivity Index .....: 11.737
Non-Corrected Log Koc (0.5213 MCI + 0.60) .....: 6.7184
4794
4795
                Fragment Correction(s):
                2 Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -2.5939
Corrected Log Koc ..... : 4.1245
4796
4797
4798
4799́
                                Estimated Koc: 1.332e+004 L/kg <=======
4800
4801
        Koc Estimate from Log Kow:
4802
               4804
4805
4806
                         2 Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -0.1312
4807
                Corrected Log Koc .....: 3.4600
4808
4809
                                Estimated Koc: 2884 L/kg <=======
4810
4813
4814
      HYDROWIN Program (v2.00) Results:
4815
4816
      SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
      CHEM: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
4817
4818
      MOL FOR: C20 H26 O4
4819
      MOL WT : 330.43
                    ----- HYDROWIN v2.00 Results -----
      NOTE: Fragment(s) on this compound are NOT available from the fragment
           library. Substitute(s) have been used!!! Substitute R1, R2, R3,
          or R4 fragments are marked with double astericks "**"
4826
4827
      ESTER: R1-C(=0)-0-R2
                                            ** R1: -Phenyl
                                               R2: -cyclohexyl
       NOTE: Ortho-position fragments(s) on Phenyl ring(s) are NOT CONSIDERED!!
4830
       Kb hydrolysis at atom # 2: 9.417E-003 L/mol-sec
4831
                                               R1: -Phenyl
R2: -cyclohexyl
      ESTER: R1-C(=0)-0-R2
4833
4834
       Kb hydrolysis at atom # 15: 9.417E-003 L/mol-sec
4835
       Total Kb for pH > 8 at 25 deg C : 1.883E-002 L/mol-sec
4836
       Kb Half-Life at pH 8: 1.166 years
Kb Half-Life at pH 7: 11.662 years
4837
4838
```

```
4841
4842
4843
        BCFBAF Program (v3.01) Results:
4844
4845
        SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
4846
        CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
        MOL FOR: C20 H26 O4
MOL WT: 330.43
4847
4848
4849
        ----- BCFBAF v3.01 -----
4850
4851
        Summary Results:
          Log BCF (regression-based estimate): 2.85 (BCF = 703 L/kg wet-wt)
Biotransformation Half-Life (days): 0.159 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 1.83 (BAF = 67.1 L/kg wet-wt)
4852
4853
4854
4855
        Log Kow (experimental): not available from database
        Log Kow used by BCF estimates: 4.82 (user entered)
4856
4857
4858
        Equation Used to Make BCF estimate:
4859
           Log BCF = 0.6598 \log Kow - 0.333 + Correction
4860
4861
               Correction(s):
4862
                No Applicable Correction Factors
4863
4864
           Estimated Log BCF = 2.847 (BCF = 703.5 L/kg wet-wt)
4865
4866
        ______
        Whole Body Primary Biotransformation Rate Estimate for Fish:
4867
        4868
4869
4870
         TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
4871
4872
       487\bar{3}
4874
4875
4876
4877
4878
4879
4880
        _____+__+__+__+
         RESULT | LOG Bio Half-Life (days) | -0.7986
RESULT | Bio Half-Life (days) | 0.159
NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C |
4881
4882
4883
4884
        4885
4886
        Biotransformation Rate Constant:
         kM (Rate Constant): 4.359 /day (10 gram fish)
kM (Rate Constant): 2.451 /day (100 gram fish)
kM (Rate Constant): 1.378 /day (1 kg fish)
kM (Rate Constant): 0.7752 /day (10 kg fish)
4887
4888
4889
4890
4891
4892
        Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
           Estimated Log BCF (upper trophic) = 1.827 (BCF = 67.13 L/kg wet-wt) Estimated Log BAF (upper trophic) = 1.827 (BAF = 67.13 L/kg wet-wt) Estimated Log BCF (mid trophic) = 1.959 (BCF = 90.99 L/kg wet-wt) Estimated Log BAF (mid trophic) = 1.962 (BAF = 91.63 L/kg wet-wt) Estimated Log BCF (lower trophic) = 1.999 (BCF = 99.71 L/kg wet-wt) Estimated Log BAF (lower trophic) = 2.031 (BAF = 107.3 L/kg wet-wt)
4893
4894
4895
4896
4897
4898
4899
4900
        Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
           Estimated Log BCF (upper trophic) = 3.758 (BCF = 5725 L/kg wet-wt)
Estimated Log BAF (upper trophic) = 4.731 (BAF = 5.377e+004 L/kg wet-wt)
4901
4902
4903
4904
```

Volatilization From Water

Chemical Name: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

330.43 g/mole Molecular Weight Water Solubility 1.48 ppm Vapor Pressure 8.69E-007 mm Hg

4907 4908

4909 4910 4911

4912 4913

4914

4915

4916

4925

4928 4929

4930 4931

4932

4933 4934

4942 4943 4944

4945

4946

4947

4948

4949 4950

4951 4952

Henry's Law Constant: 9.45E-008 atm-m3/mole (entered by user)

	RIVER	LAKE
Water Depth (meters): Wind Velocity (m/sec): Current Velocity (m/sec):	1 5 1	1 0.5 0.05
HALF-LIFE (hours) :	1.127E+004	1.231E+005

HALF-LIFE (days): 469.5 5129 HALF-LIFE (years): 1.286 14.04

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

(using 10000 hr Bio P,A,S)

PROPERTIES OF: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester

Molecular weight (g/mol)	330.43
Aqueous solubility (mg/l)	1.48
Vapour pressure (Pa)	0.000115857
(atm)	1.14342E-009
(mm Hg)	8.69E-007
Henry 's law constant (Atm-m3/mol)	9.446E-008
Air-water partition coefficient	3.86313E-006
Octanol-water partition coefficient (Kow)	66069.4
Log Kow	4.82
Biomass to water partition coefficient	13214.7
Tomponoturo [dog C]) [

Temperature [deg C] Biodeg rate constants (h^-1), half life in biomass (h) and in 2000 mg/L MLSS (h):

0.00 -Primary tank 9635.43 10000.00 -Aeration tank -Settling tank 0.00 9635.43 10000.00 9635.43 10000.00 0.00

STP Overall Chemical Mass Balance:

	g/h	mol/h	percent
Influent	1.00E+001	3.0E-002	100.00
Primary sludge Waste sludge Primary volatilization Settling volatilization Aeration off gas	4.35E+000 2.70E+000 1.41E-005 3.44E-005 8.47E-005	1.3E-002 8.2E-003 4.3E-008 1.0E-007 2.6E-007	43.54 27.02 0.00 0.00 0.00
Primary biodegradation Settling biodegradation Aeration biodegradation	1.32E-002 3.53E-003 4.65E-002	4.0E-005 1.1E-005 1.4E-004	0.13 0.04 0.47
Final water effluent	2.88E+000	8.7E-003	28.81
Total removal Total biodegradation	7.12E+000 6.32E-002	2.2E-002 1.9E-004	71.19 0.63

STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility

```
4974
       _____
4975
          (using Biowin/EPA draft method)
4976
       PROPERTIÉS OF: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
4977
4978
       Molecular weight (g/mol)
4979
                                                                 1.48
       Aqueous solubility (mg/l)
4980
       Vapour pressure (Pa)
                                                                 0.000115857
4981
                                                                 1.14342E-009
                        (atm)
4982
                        (mm Hg)
                                                                 8.69E-007
4983
       Henry 's law constant (Atm-m3/mol)
                                                                 9.446E-008
4984
       Air-water partition coefficient
                                                                 3.86313E-006
4985
       Octanol-water partition coefficient (Kow)
                                                                 66069.4
4986
                                                                 4.82
4987
       Biomass to water partition coefficient
                                                                 13214.7
4988
       Temperature [deg C]
                                                                 25
4989
       Biodeg rate constants (h^{-1}), half life in biomass (h) and in 2000 mg/L MLSS (h):
4990
                                      0.01
                 -Primary tank
                                                    96.35
                                                                   100.00
4991
                                                     9.64
                                        0.07
                                                                    10.00
                 -Aeration tank
4992
                                                     9.64
                 -Settling tank
                                        0.07
                                                                    10.00
4993
4994
        STP Overall Chemical Mass Balance:
4995
4996
                                      g/h
                                                         mol/h
                                                                        percent
4997
4998
       Influent
                                                        3.0E-002
                                                                        100.00
                                     1.00E+001
4999
5000
                                     3.85E+000
                                                                        38.51
       Primary sludge
                                                       1.2E-002
5001
                                     2.37E-001
       Waste sludge
                                                       7.2E-004
                                                                         2.37
5002
       Primary volatilization
                                                                         0.00
                                    1.25E-005
                                                        3.8E-008
5003
                                     3.02E-006
       Settling volatilization
                                                        9.1E-009
                                                                          0.00
5004
       Aeration off gas
                                     7.61E-006
                                                        2.3E-008
                                                                          0.00
5005
5006
       Primary biodegradation
                                     1.17E+000
                                                        3.5E-003
                                                                        11.68
5007
       Settling biodegradation
                                     3.10E-001
                                                        9.4E-004
                                                                         3.10
5008
       Aeration biodegradation
                                     4.18E+000
                                                        1.3E-002
                                                                         41.81
5009
5010
       Final water effluent
                                     2.53E-001
                                                       7.7E-004
                                                                          2.53
5011
5012
       Total removal
                                     9.75E+000
                                                        2.9E-002
                                                                        97.47
5013
       Total biodegradation
                                     5.66E+000
                                                       1.7E-002
                                                                        56.59
5014
        (** Total removal recommended maximum is 95 percent)
5015
5016
       Level III Fugacity Model (Full-Output): MCI Method
5017
5018
       Chem Name : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
5019
5020
         Molecular Wt: 330.43
         Henry's LC: 9.45e-008 atm-m3/mole (user-entered)
Vapor Press: 8.69e-007 mm Hg (user-entered)
Liquid VP: 2.21e-006 mm Hg (super-cooled)
Melting Pt: 66 deg C (user-entered)
5021
5022
5023
50\overline{24}
5025
                     : 4.82 (user-entered)
         Log Kow
5026
         Soil Koc
                      : 1.33e+004 (KOCWIN MCI method)
5027
5028
                                  Half-Life
                   Mass Amount
                                                Emissions
5029
                    (percent)
                                      (hr)
                                                  (kg/hr)
                                                   1000
5030
                                      10.6
                     0.228
          Air
5031
          Water
                     13.2
                                      900
                                                   1000
5032
          Soil
                     76.4
                                      1.8e + 003
                                                    1000
5033
          Sediment
                    10.2
                                      8.1e+003
5034
5035
                     Fugacity
                                 Reaction
                                              Advection
                                                           Reaction
                                                                       Advection
                                 (kg/hr)
                                                                        (percent)
5036
                      (atm)
                                                           (percent)
                                               (kg/hr)
                     5.06e-012
                                  630
                                               96.2
5037
          Air
                                                            21
                                                                         3.21
5038
                    7.79e-013
                                                            14.3
          Water
                                  429
                                               557
                                                                        18.6
                    1.6e-013
5039
                                  1.24e+003
                                                            41.4
                                               0
                                                                        0
          Soil
5040
                                  36.7
                                                            1.22
          Sediment 9.55e-013
                                               8.57
                                                                        0.286
```

```
5041
5042
          Persistence Time: 1.41e+003 hr
504\overline{3}
                              1.81e+003 hr
          Reaction Time:
5044
          Advection Time:
                              6.37e+003 hr
5045
                              77.9
          Percent Reacted:
5046
           Percent Advected: 22.1
5047
5048
          Water Compartment Percents:
5049
5050
                                    Half-Life
                                                  Emissions
                   Mass Amount
5051
                    (percent)
                                       (hr)
                                                    (kg/hr)
                     0.228
13.2
5052
                                                      1000
          Air
                                       10.6
5053
                                                      1000
          Water
                                       900
5054
                        (12.9)
             water
5055
                        (0.0426)
             biota
5056
             suspended sediment (0.258)
5057
                     76.4
                                       1.8e + 003
                                                      1000
5058
                    10.2
                                       8.1e+003
          Sediment
                                                      O
5059
          Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin): Air: 10.58
5060
5061
5062
                         900
              Water:
5063
              Soil:
                         1800
5064
              Sediment: 8100
5065
                Biowin estimate: 2.749 (weeks-months)
5066
5067
          Advection Times (hr):
5068
                         100
              Air:
5069
              Water:
                         1000
5070
              Sediment: 5e+004
5071
5072
5073
       Level III Fugacity Model (Full-Output): EQC Default
5074
5075
                       : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
         Chem Name
5076
         Molecular Wt: 330.43
5077
                      : 9.45e-008 atm-m3/mole (user-entered)
         Henry's LC
5078
         Vapor Press: 8.69e-007 mm Hg (user-entered)
5079
         Liquid VP
                       : 2.21e-006 mm Hg (super-cooled)
5080
                      : 66 deg C (user-entered)
         Melting Pt
5081
         Log Kow
Soil Koc
                       : 4.82
                               (user-entered)
5082
                       : 2.71e+004
                                    (EQC Model Default)
5083
5084
                                    Half-Life
                   Mass Amount
                                                  Emissions
                                                   (kg/hr)
5085
                     (percent)
                                       (hr)
5086
                                       10.6
                                                      1000
          Air
                      0.209
5087
                     11.6
                                       900
                                                      1000
          Water
                                       1.8e+003
5088
                      70.3
          Soil
                                                      1000
5089
                     17.9
                                       8.1e+003
          Sediment
5090
5091
                                                                           Advection
                      Fugacity
                                   Reaction
                                                Advection
                                                             Reaction
5092
                                   (kg/hr)
                                                 (kg/hr)
                                                             (percent)
                                                                           (percent)
                       (atm)
5093
                      5.05e-012
          Air
                                    630
                                                 96.2
                                                              21
                                                                            3.21
                                                                            17.8
5094
                      7.3e-013
                                                              13.7
          Water
                                    411
                                                 533
5095
                                    1.24e+003
           Soil
                      7.88e-014
                                                 0
                                                              41.4
5096
          Sediment
                     9.02e-013
                                    70.3
                                                 16.4
                                                              2.34
                                                                            0.548
5097
5098
          Persistence Time: 1.53e+003 hr
5099
          Reaction Time:
                              1.95e+003 hr
5100
                              7.11e+003 hr
          Advection Time:
5101
          Percent Reacted:
                              78.5
           Percent Advected: 21.5
5102
5103
5104
          Water Compartment Percents:
5105
5106
                                    Half-Life
                                                  Emissions
                   Mass Amount
5107
                    (percent)
                                       (hr)
                                                   (kg/hr)
```

```
December 2024
5108
                                          10.6
           Air
                       0.209
                                                         1000
5109
           Water
                       11.6
                                          900
                                                         1000
5110
                          (11.1)
             water
5111
                          (0.0367)
              biota
5112
              suspended sediment (0.452)
5113
           soil 70.3
                                          1.8e + 003
                                                         1000
5114
           Sediment 17.9
                                          8.1e+003
5115
5116
           Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin): Air: 10.58
5117
5118
5119
5120
                          900
               Water:
               Soil:
                           1800
               Sediment: 8100
5121
5122
                 Biowin estimate: 2.749 (weeks-months)
51\overline{23}
           Advection Times (hr):
5124
               Air:
                          100
51\overline{2}5
                          1000
               Water:
5126
               Sediment: 5e+004
```

A.9 Atmospheric Oxidation Rate (AOPWIN)

5127

5154

5169

```
5128
        Run Date: 2024-06-21
5129
5130
        SMILES: 0=C(0C(CCCC1)C1)c(c(ccc2)C(=0)0C(CCCC3)C3)c2
5131
5132
5133
5134
        CHEM : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
        MOL FOR: C20 H26 O4 MOL WT : 330.43
                     ----- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) ------
        Hydrogen Abstraction = 23.5226 E-12 cm3/molecule-sec
Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
5135
5136
5137
5138
        Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
5139
        **Addition to Aromatic Rings = 0.7492 E-12 cm3/molecule-sec
5140
        Addition to Fused Rings
                                        = 0.0000 E-12 cm3/molecule-sec
5141
5142
            OVERALL OH Rate Constant = 24.2718 \text{ E}-12 \text{ cm}3/\text{molecule-sec}
HALF-LIFE = 0.441 \text{ Days} (12-\text{hr day}; 1.5E6 \text{ OH/cm}3)
5143
            HALF-LIFE =
5144
            HALF-LIFE =
                              5.288 Hrs
5145
        ..... ** Designates Estimation(s) Using ASSUMED Value(s)
5146
        ----- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) -----
5147
5148
                           ***** NO OZONE REACTION ESTIMATION *****
5149
                           (ONLY Olefins and Acetylenes are Estimated)
5150
5151
        Experimental Database: NO Structure Matches
5153
```

A.10 Destruction and Removal in Wastewater Treatment Plants (STPWIN)

```
5155
       Run Date: 2024-06-21
5156
5157
5158
5159
       STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
           (using 10000 \text{ hr Bio P,A,S})
5160
       PROPERTIES OF: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
5161
5162
       Molecular weight (g/mol)
                                                                    330.43
       Aqueous solubility (mg/l)
5163
                                                                    1.48
5164
                                                                    0.000115857
       Vapour pressure (Pa)
5165
                         (atm)
                                                                    1.14342E-009
5166
                                                                    8.69E-007
                         (mm Hg)
5167
5168
       Henry 's law constant (Atm-m3/mol)
                                                                    9.446E-008
       Air-water partition coefficient
                                                                    3.86313E-006
```

Octanol-water partition coefficient (Kow)

66069.4

```
5170
        Log Kow
                                                                         4.82
        Biomass to water partition coefficient 13214.7
Temperature [deg C] 25
Biodeg rate constants (h^-1), half life in biomass (h) and in 2000 mg/L MLSS (h):
5171
5172
5173
5174
5175
                                       0.00
                                                        9635.43
                    -Primary tank
                                                                         10000.00
                                                        9635.43
                                            0.00
                                                                         10000.00
                    -Aeration tank
5176
                    -Settling tank
                                            0.00
                                                        9635.43
                                                                         10000.00
5177
5178
         STP Overall Chemical Mass Balance:
5179
5180
5181
5182
5183
5184
                                                               mol/h
                                                                                 percent
        Influent
                                         1.00E+001
                                                              3.0E-002
                                                                                 100.00
        Primary sludge
                                         4.35E+000
                                                              1.3E-002
                                                                                 43.54
5185
        Waste sludge
                                         2.70E+000
                                                              8.2E-003
                                                                                 27.02
5186
5187
        Primary volatilization
                                     1.41E-005
3.44E-005
                                                              4.3E-008
                                                                                 0.00
                                                              1.0E-007
        Settling volatilization
                                                                                  0.00
5188
                                         8.47E-005
        Aeration off gas
                                                              2.6E-007
                                                                                  0.00
5189
5190
5191
                                         1.32E-002
3.53E-003
        Primary biodegradation
                                                              4.0E-005
                                                                                  0.13
        Settling biodegradation
                                                              1.1E-005
                                                                                  0.04
5192
5193
        Aeration biodegradation
                                         4.65E-002
                                                              1.4E-004
                                                                                  0.47
5194
        Final water effluent
                                         2.88E+000
                                                              8.7E-003
                                                                                 28.81
5195
5196
                                                              2.2E-002
                                         7.12E+000
        Total removal
                                                                                 71.19
5197
        Total biodegradation
                                         6.32E-002
                                                              1.9E-004
                                                                                  0.63
5198
5199
5200
5201
        STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility
5202
5203
           (using Biowin/EPA draft method)
5204
        PROPERTIES OF: 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
5205
5206
        Molecular weight (g/mol)
                                                                         330.43
5207
5208
5209
        Aqueous solubility (mg/l)
                                                                         1.48
        Vapour pressure (Pa)
                                                                         0.000115857
                                                                         1.14342E-009
                           (atm)
5210
5211
5212
                           (mm Hg)
                                                                         8.69E-007
        Henry 's law constant (Atm-m3/mol)
                                                                         9.446E-008
        Air-water partition coefficient
                                                                         3.86313E-006
5212
5213
5214
        Octanol-water partition coefficient (Kow)
                                                                         66069.4
        Log Kow
                                                                         4.82
5214
5215
5216
5217
5218
5219
5220
        Biomass to water partition coefficient
                                                                         13214.7
        Temperature [deg C]
                                                                         25
        Biodeg rate constants (h^-1), half life in biomass (h) and in 2000 mg/L MLSS (h):
                    -Primary tank 0.01
                                                          96.35
                                                                           100.00
                    -Aeration tank
                                            0.07
                                                            9.64
                                                                            10.00
                    -Settling tank
                                                            9.64
                                                                            10.00
                                            0.07
5221
5222
         STP Overall Chemical Mass Balance:
5\overline{2}\overline{2}
5\overline{2}\overline{2}4
                                                               mol/h
                                                                                 percent
5224
5225
5226
5227
5228
5229
        Influent
                                         1.00E+001
                                                              3.0E-002
                                                                                 100.00
        Primary sludge
Waste sludge
                                                                                 38.51
                                         3.85E+000
                                                              1.2E-002
                                                              7.2E-004
                                                                                  2.37
                                         2.37E-001
5230
5231
5232
                                         1.25E-005
                                                              3.8E-008
                                                                                  0.00
        Primary volatilization
        Settling volatilization
                                         3.02E-006
                                                              9.1E-009
                                                                                  0.00
        Aeration off gas
                                         7.61E-006
                                                              2.3E-008
                                                                                  0.00
5\overline{2}3\overline{3}
5234
        Primary biodegradation
                                         1.17E+000
                                                              3.5E-003
                                                                                 11.68
                                        3.10E-001
5235
        Settling biodegradation
                                                              9.4E-004
                                                                                  3.10
                                                                                 41.81
5236
        Aeration biodegradation
                                         4.18E+000
                                                              1.3E-002
```

```
5238
5238
5239
        Final water effluent
                                        2.53E-001
                                                               7.7E-004
                                                                                    2.53
5\overline{240}
        Total removal
                                          9.75E+000
                                                                2.9E-002
                                                                                   97.47
        5241
                                                                                   56.59
5242
         (** Total removal recommended maximum is 95 percent)
        A.11 Bioaccumulation Potential (BCFBAF)
5243
5244
        Run Date: 2024-07-02
5245
5246
5247
        SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3
        CHEM : Dicyclohexyl Phthalate
5248
        MOL FOR: C20 H26 O4
5249
        MOL WT : 330.43
5\bar{2}50
                        ------ BCFBAF v3.01 -----
5251
5252
5253
5254
5255
5256
5257
5258
5259
        Summary Results:
          Log BCF (regression-based estimate): 2.85 (BCF = 703 L/kg wet-wt)
Biotransformation Half-Life (days): 0.159 (normalized to 10 g fish)
Log BAF (Arnot-Gobas upper trophic): 1.83 (BAF = 67.1 L/kg wet-wt)
        BCF (Bioconcentration Factor):
        _____
        Log Kow (estimated) : 6.20
Log Kow (experimental): not available from database
5260
5261
        Log Kow used by BCF estimates: 4.82 (user entered)
5262
5263
5264
        Equation Used to Make BCF estimate:
            Log BCF = 0.6598 \log Kow - 0.333 + Correction
5265
5266
5267
               Correction(s):
                 No Applicable Correction Factors
5268
5269
            Estimated Log BCF = 2.847 (BCF = 703.5 L/kg wet-wt)
5279
5270
5271
5272
5273
5274
        ______
        Whole Body Primary Biotransformation Rate Estimate for Fish:
        5\overline{275}
         TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
5276
5277
5278
        5279
5\overline{2}80
5281
5282
5283
5284
5285
5286
5287
5288
          RESULT | LOG Bio Half-Life (days) | RESULT | Bio Half-Life (days) | NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C
                                                                                          | -0.7986
                                                                                             0.159
5289
        52<u>9</u>0
5291
5292
        Biotransformation Rate Constant:
         kM (Rate Constant): 4.359 /day (10 gram fish)
kM (Rate Constant): 2.451 /day (100 gram fish)
kM (Rate Constant): 1.378 /day (1 kg fish)
kM (Rate Constant): 0.7752 /day (10 kg fish)
5293
5\overline{2}94
5295
5296
5<u>2</u>97
        Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates):
           Estimated Log BCF (upper trophic) = 1.827 (BCF = 67.13 L/kg wet-wt) Estimated Log BAF (upper trophic) = 1.827 (BAF = 67.13 L/kg wet-wt) Estimated Log BCF (mid trophic) = 1.959 (BCF = 90.99 L/kg wet-wt) Estimated Log BAF (mid trophic) = 1.962 (BAF = 91.63 L/kg wet-wt)
5298
5299
```

December 2024

5302	Estimated Log BCF (lower trophic) = 1.999 (BCF = 99.71 L/kg wet-wt)
5303	Estimated Log BAF (lower trophic) = 2.031 (BAF = 107.3 L/kg wet-wt)
5304	
5305	Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero):
5306	Estimated Log BCF (upper trophic) = 3.758 (BCF = 5725 L/kg wet-wt)
5307	Estimated Log BAF (upper trophic) = 4.731 (BAF = 5.377e+004 L/kg wet-wt)

A.12 Biodegradation Potential (BIOWIN)

5310 SMILES: C1CCC(CC1)OC(=0)c2cccc2C(=0)OC3CCCCC3 CHEM : Dicyclohexyl Phthalate

MOL FOR: C20 H26 O4 MOL WT : 330.43

Run Date: 2024-06-12.

5308

5309

5313

5314

5315

5318

5319 5320

5344 5345

5346

5360

5363 5364 5365 ----- BIOWIN v4.10 Results -----

Biowin1 (Linear Model Prediction) : Biodegrades Fast Biowin2 (Non-Linear Model Prediction): Biodegrades Fast

Biowin3 (Ultimate Biodegradation Timeframe): Weeks-Months
Biowin4 (Primary Biodegradation Timeframe): Days
Biowin5 (MITI Linear Model Prediction): Readily Degradable
Biowin6 (MITI Non-Linear Model Prediction): Readily Degradable
Biowin7 (Anaerobic Model Prediction): Does Not Biodegrade Fast
Ready Biodegradability Prediction: NO

		l	-	I
TYPE	NUM	Biowin1 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag MolWt Const	2 * *	Ester [-C(=0)-O-C] Molecular Weight Parameter Equation Constant	0.1742	0.3484 -0.1573 0.7475
RESULT		Biowin1 (Linear Biodeg Probability)	 -1	0.9386
				r
TYPE	NUM	Biowin2 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag MolWt	2 *	Ester [-C(=0)-O-C] Molecular Weight Parameter	4.0795	8.1590 -4.6921
RESULT		Biowin2 (Non-Linear Biodeg Probability)	- 	0.9985
		T	-T	r

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

TYPE	NUM	Biowin3 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag MolWt Const	2 * *	Ester [-C(=O)-O-C] Molecular Weight Parameter Equation Constant	0.1402	0.2804 -0.7302 3.1992
RESULT		Biowin3 (Survey Model - Ultimate Biodeg)	+====== 	2.7494
			+======	r=======
TYPE	NUM	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
			+	

Frag 2	Ester [-C(=0)-O-C]	0.2290	0.4579
MolWt *	Molecular Weight Parameter		-0.4767
Const *	Equation Constant		3.8477
RESULT	Biowin4 (Survey Model - Primary Biodeg)	 	3.8289

Result Classification: 5.00 -> hours 4.00 -> days 3.00 -> weeks (Primary & Ultimate) 2.00 -> months 1.00 -> longer

TYPE	+ NUM :	+Biowin5 FRAGMENT DESCRIPTION	+	VALUE
Frag Frag Frag Frag MolWt Const	•	Ester [-C(=0)-O-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Molecular Weight Parameter Equation Constant	0.2319 0.0004 0.0141 0.0079	0.4638 0.0016 0.1411 0.0158 -0.5211 0.5544
RESU	=====- JLT 	Biowin5 (MITI Linear Biodeg Probability)	+======= !	0.6556

TYPE	NUM	Biowin6 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag Frag Frag Frag MolWt	2 4 10 2 *	Ester [-C(=0)-O-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Molecular Weight Parameter	1.5833 0.0342 0.1206 0.0294	3.1665 0.1368 1.2058 0.0589 -5.7164
RESULT		Biowin6 (MITI Non-Linear Biodeg Probability)		0.6257

A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable A Probability Less Than 0.5 indicates --> NOT Readily Degradable

		L	L	L
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag Frag Frag Frag Const	2 4 10 2	Ester [-C(=0)-O-C] Aromatic-H -CH2- [cyclic] -CH - [cyclic] Equation Constant	0.1719 -0.0954 -0.1200 0.0395	0.3437 -0.3817 -1.2001 0.0789 0.8361
RESULT		Biowin7 (Anaerobic Linear Biodeg Prob)		-0.3232
		ı ————————————————————————————————————		

A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast

Ready Biodegradability Prediction: (YES or NO)

Criteria for the YES or NO prediction: If the Biowin3 (ultimate survey model) result is "weeks" or faster (i.e. "days", "days to weeks", or "weeks" AND the Biowin5 (MITI linear model) probability is >= 0.5, then the prediction is YES (readily biodegradable). If this condition is not satisfied, the prediction is NO (not readily biodegradable). This method is based on application of Bayesian analysis to ready biodegradation data (see Help). Biowin5 and 6 also predict ready biodegradability, but for degradation in the OECD301C test only; using data from the Chemicals Evaluation and Research Institute Japan (CERIJ) database.

Appendix B KEY FINDINGS OF RELEVANT INTERNATIONAL PUBLICATIONS

B.1 Indoor Air and Dust

Six international studies surveyed DCHP concentrations in indoor air and dust. A brief summary of each study is provided below:

- A 2009 survey of six Tokyo households found DCHP in all surveyed homes at concentrations ranging from non-detect (n.d.) to 170 ng/m³ (Otake et al., 2001).
- A small 2012 survey of six Sapporo households identified two homes where concentrations measured in bedrooms were 14 and 4 ng/m³ with no DCHP recorded in any of the living rooms (Takeuchi et al., 2014).
- A 2016 survey of 97 Vietnamese locations including schools, offices, homes, laboratories, and hair salons recorded DCHP concentrations in 87 percent of indoor air samples with a (n.d.–398 ng/m³) (Tran et al., 2017). The concentrations in this study were skewed with a handful of high concentration samples driving the mean above the median by an order of magnitude with a mean concentration of 32.4 ng/m³ and the median concentration of 4.54 ng/m³. The skew to higher concentrations of DCHP was attributed to DCHP used in hair salons and laboratories (Tran et al., 2017).
- A 2019 survey of 85 Japanese households identified DCHP in 41 percent of sampled households at concentrations ranging from n.d. to 3.0 ng/m³ (Yoshida et al., 2020).
- A 2020 survey of indoor air at 24 primary schools in Barcelona identified DCHP in several samples with a mean atmospheric concentration of 110 ± 93 ng/m³. Elevated concentrations in downtown regions were observed with a mean concentration of 95 ± 13 ng/m³ (traffic) (van Drooge et al., 2020). The highest DCHP air concentrations were attributed to formation of DCHP as a combustion byproduct resulting from vehicle emissions (van Drooge et al., 2020). Concentrations of DCHP were an order of magnitude higher than outdoor DCHP concentration in both congested (12 ± 3 ng/m³ indoor, 95 ± 13 ng/m³ outdoor) and non-congested (9 ± 3 ng/m³ indoor, 110 ± 93 ng/m³ outdoor) areas (van Drooge et al., 2020).
- A 2019 survey of 30 newly constructed homes, 30 older homes, and 30 offices in China identified DCHP with average gas-phase concentrations ranging including 699 ng/m³ (n.d–1923 ng/m³) in newly constructed homes, 512 ng/m³ (< 37.2–787 ng/m³) in existing homes, and 377 ng/m³ (< 7.2–1,257 ng/m³) in office. DCHP was also detected in the dust and air particulate with a mean concentration of 627 ng/m³ (<29.67–1,208 ng/m³) in newly constructed homes, 667 ng/m³ (<29.67–995 ng/m³) in existing homes, and 502 ng/m³ (71–1,197 ng/m³) in offices (Ouyang et al., 2019).

B.2 Outdoor Air and Dust

Five international studies surveyed DCHP concentrations in outdoor air and dust. A summary of each study is provided below:

• A 2012 survey of indoor air at 24 primary schools in Barcelona identified DCHP in of samples with a mean outdoor atmospheric concentration of 9 ± 3 ng/m³ (background) with elevated concentrations in downtown regions with a mean concentration of 12 ± 3 ng/m³ (traffic) (van Drooge et al., 2020). The highest DCHP air concentrations were attributed to high emissions from vehicles with the highest concentrations found in congested downtown regions (van Drooge

- 5468 <u>et al., 2020</u>). Concentrations of DCHP were an order of magnitude lower than indoor DCHP concentration in both congested (95 \pm 13 ng/m³) and non-congested (110 \pm 93 ng/m³) areas (van Drooge et al., 2020).
- A 2011 survey of air quality around Lake Chaohu in China demonstrated median DCHP concentrations of 1.55 pg/m³ (<1–3.66 pg/m³, n = 7) and 0.771 pg/m³ (<1–1.17 pg/m³, n = 8) in lakeside and urban regions, respectively (HEW, 2019).
 - A 2016 survey of 70 Turkish industrial and residential sites identified DCHP in 100 percent of indoor and outdoor dust samples with concentrations of 21.8 ± 38.8 mg/kg in indoor dust and 0.39 ± 0.61 mg/kg in outdoor dust (<u>Başaran et al., 2020</u>). Concentrations of all phthalates were highest in urban developed regions followed by industrial sites, near-road sites, and lowest concentrations in rural sites (<u>Başaran et al., 2020</u>).
 - A 2018 survey of DCHP around a single lake in South Korea identified DCHP in both outdoor air and dust (n = 4); DCHP was not detected in air samples but was detected in outdoor dust with a median concentration of 0.03 ng/m³ (<0.02–0.03 ng/m³), making up all appreciable DCHP in the atmospheric samples (Lee et al., 2019).
 - A 2019 survey of 30 outdoor sites in China identified DCHP in both air and air particulate with a mean concentration of 107 ng/m³ (n.d.–459 ng/m³) in air and 130 ng/m³ (n.d.–485 ng/m³) on dust (Ouyang et al., 2019).

B.3 Surface Water

Seven international studies have reported DCHP in surface water and suspended particulate. A summary of the findings for each study is provided below:

- A 2016 of 22 aquaculture ponds around China identified DCHP ranging from 0.02 to 0.25 μg/m³ with sediment concentrations ranging from 80 to 590 μg/kg at the same locations (Cheng et al., 2019).
- A 2019 Chinese survey of an archipelago in the Tropical Western Pacific Ocean identified DCHP in seamount surface water samples ranging from 1.09 to 7.29 ng/L (n = 18) (Zhang et al., 2019a).
- A 2019 survey of one lake consisting of 47 samples in South Korea identified DCHP in 2 percent of samples with concentrations ranging from less than 0.02 to 0.07 μg/L. DCHP was identified in 6.4 percent of benthic sediment samples in the same lake with a concentration ranging from less than 0.41 to 18.8 μg/kg. DCHP was also identified in 13.3 percent of fish tissue (n = 30) with a concentration range from less than 0.22 to 21.9 μg/kg (Lee et al., 2019).
- A 2006 survey of Guangzhous, China identified 7 percent (n = 15) of urban lake samples with concentrations ranging from less than the MDL to $0.076 \,\mu\text{g/L}$ and in 53 percent of benthic sediments with concentrations ranging from less than the MDL to $0.22 \,\mu\text{g/g}$ dw (Zeng et al., 2008a). The MDL was not provided.
- A 2017 survey of five sites in Kuwait's coastal waters identified DCHP in coastal samples ranging in concentrations from 0.2 to 9.4 ng/L. DCHP was also identified in coastal sediment samples at concentrations from 68.9 to 1,195.2 μg/kg. Sampling sites were in close duration to wastewater plants with known emissions of phthalate-containing effluent with effluent containing concentrations of total phthalates ranging from 1.5 to 77 μg/L (0.01–1.14 μg/L DCHP) (Saeed et al., 2017).

5510 Another 2005 survey of various surface water, municipal wastewater, and industrial wastewater 5511 treatment plants measured DCHP across The Netherlands. DCHP was identified in 50 percent of 5512 untreated municipal wastewater (n = 12) ranging from less than 11 to 210 ng/L with DCHP 5513 detected in 22 percent of effluent samples with concentration ranging from 2 to 20 ng/L. DCHP 5514 was identified in 80 percent of untreated industrial wastewater with concentrations ranging from less than 5 to 19,000 ng/L. DCHP was round in no rainwater samples (n = 3) but was detected in 5515 5516 33 percent of surface water samples with concentrations ranging from less than 3 to 60 ng/L, 47 5517 percent of suspended particulate samples at the same sites at concentrations ranging from less than 2 to 1,300 ng/g dw, and in 19 percent of benthic sediment samples at concentrations ranging 5518 5519 from less than 2 to 11 ng/g dw (Vethaak et al., 2005).

B.4 Sediment

- 5521 Three international studies identified DCHP in suspended sediments originating from China, The
- Netherlands, and Germany. The measured concentration ranges of DCHP measured in suspended 5522
- 5523 sediment are listed below:
- 5524 • 1.3 to 11.4 ng/l in China (Zhao et al., 2020);
 - 41 ng/l in The Netherlands (Vethaak et al., 2005); and
 - 14 to 15 ng/l in Germany (Nagorka and Koschorreck, 2020).
- 5527 Several studies reported DCHP measured in benthic sediments originating from China, Iran, South
- 5528 Korea, Kuwait, and The Netherlands; DCHP concentration ranges reported for each region are listed
- 5529 below:

5520

5525 5526

5534

- 5530 • 0.01 to 590 ng/g in China (Hu et al., 2020; Cheng et al., 2019; Mi et al., 2019; Sun et al., 2013; 5531 Zeng et al., 2008a);
- 5532 • 290 to 2,300 ng/g in Iran (Arfaeinia et al., 2019);
- 0.7 ng/g in South Korea (Lee et al., 2019); 5533
 - 68.9 to 1,195.2 ng/g in Kuwait (Saeed et al., 2017); and
- 5535 39 ng/g in The Netherlands (Vethaak et al., 2005).

B.5 Soil 5536

- 5537 Five chinese studies identified DCHP in soil. Concentrations ranged from 0.0058 to 11.8 µg/g dw of
- 5538 DCHP in soil has been measured in China (Zhang et al., 2019b; Niu et al., 2014; Liu et al., 2010; Zeng
- 5539 et al., 2009; Zeng et al., 2008b).

5540 **B.6** Biosolids

- Three international studies have been identified pertaining to DCHP concentrations in wastewater 5541
- 5542 biosolids:
- 5543 A survey of wastewater removal of phthalates in China identified DCHP in 100 percent of 5544 samples collected with concentrations ranging from 7.98 to 14.41 µg/L with DCHP making up between 6 to 19 percent of overall phthalate concentrations (Wu et al., 2019). Removal 5545 5546 efficiencies ranged from 69 to 98 percent between the three plants; DCHP was detected in sludge in two of the three facilities with an average concentration of 0.31 ± 0.20 mg/kg dry weight 5547 accounting to 10 to 20 percent of the initial DCHP mass lost to biosolids sorption during 5548
- 5549 wastewater treatment (Wu et al., 2019). Destruction of DCHP accounted for 51 to 56 percent of
- 5550 initial DCHP mass lost to destruction (Wu et al., 2019).
- 5551 A 2019 Chinese survey of wastewater sludge from 46 wastewater treatment plants found DCHP

- in 57 percent of sampled a mean DCHP concentration of 0.0093 ng/kg (0.0014–0.0836 mg/kg) making up less than 1 percent of the total phthalate concentration in biosolids (Zhu et al., 2019).
- A 2013 survey of 25 Chinese wastewater plants resulted identified DCHP in 100 percent of sludge sampled (n = 25) with a mean concentration of 0.10 mg/kg (0.039–0.19 mg/kg out of the 123 mg/kg (22.6–1,350 mg/kg) total phthalates, accounting for 0.08 percent of total phthalates present in sludge samples on average (Meng et al., 2014).

B.7 Landfills

No international studies were identified related to DCHP in landfill or landfill leachate.

B.8 Groundwater

Three international studies were identified related to DCHP in groundwater originating in China. Key points related to DCHP in groundwater extracted from the studies are summarized below:

- A 2019 survey of three wastewater treatment plants in China identified DCHP in 100 percent of the wastewater influent samples with 30 to 33 percent of phthalates making it through the wastewater treatment plant into wastewater effluent releasing an estimate 2.1 to 11.0 kg phthalates/day (0.17–3.84 μg/L) into nearby surface waters (Wu et al., 2019).
- A 2000 field study in China collected 47 shallow (0–20 cm) and 47 deep (150–180 cm) soil samples cover a 1,000 km² region of the Great North China Plains near a river exhibiting groundwater interactions. Although DCHP was not included in the total phthalates analysis, total phthalates in shallow soils ranged from 0.94 ± 0.99 mg/kg total phthalates in shallow soils and 0.61 ± 0.73 mg/kg total phthalates in deep soils.
- A 2007 survey of 15 sediment and pore water samples in the Guangzhou region of China identified DCHP in sorbed to sediments in 53 percent of sediment samples at concentrations ranging from undetected to 0.22 mg/kg and in 7 percent of pore water samples ranging from undetected to 0.076 g/L (Zeng et al., 2008a).
 - The increased detection frequency and higher mean concentrations in the sorbed sediment compared to the surrounding pore water aligns with the water solubility and partitioning coefficients suggesting that DCHP will largely sorb to particulate media with limited mobility in the water phase.

B.9 Wastewater Treatment

Only one study was identified pertaining to the removal of DCHP in wastewater treatment processes; The study surveyed three wastewater treatment plants in china including removal from primary treatment, biological treatment (SBR, AAOBR, and MSBR), and secondary clarification. DCHP was identified in 100 percent of samples collected from the wastewater plant with concentrations ranging from 7.98 to 14.41 μ g/L with DCHP comprising between 6 and 19 percent of overall phthalate concentrations (Wu et al., 2019). Removal efficiencies ranged from 69 to 98 percent between the three plants (Wu et al., 2019). DCHP was detected in sludge in two of the three facilities with an average concentration of 310 \pm 200 μ g/kg dry weight. DCHP, which was not degraded or sorbed to biosolids, passed through the wastewater treatment processes with residual DCHP concentrations in effluent ranging from 0.17 to 3.84 μ g/L (Wu et al., 2019). While the sample size is small and more data would be needed to draw substantial conclusions from the differences in DCHP removal efficiencies between treatment technologies, the membrane-based biological treatment technology did have a higher removal efficiency and lower DCHP residual in the effluent compared to the conventional biological treatment

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systems. Tertiary treatment, including filtration, chemical disinfection, of ultraviolet (UV) light disinfection, were not evaluated in this study.

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- Another 2005 survey of various surface water, municipal wastewater, and industrial wastewater
- 5598 treatment plants measured DCHP across The Netherlands. DCHP was identified in 50 percent of
- untreated municipal wastewater (n = 12) ranging from less than 11 to 210 ng/L with DCHP detected in
- 5600 22 percent of effluent samples with concentrations ranging from 2 to 20 ng/L. DCHP was identified in
- 5601 80 percent of untreated industrial wastewater with concentrations ranging from less than 5 to 19,000
- 5602 ng/L (Vethaak et al., 2005).

B.10 Drinking Water Treatment

- No international studies were identified related to DCHP fate or transformation during drinking water
- 5605 treatment.

B.11 Bioaccumulation Potential

- Only one international study was identified related to bioaccumulation potential of DCHP. A 2019
- survey of 1 lake consisting of 47 samples in South Korea identified DCHP in 2 percent of samples with
- 5609 concentrations ranging from less than 0.02 to 0.07 µg/L. DCHP was identified in 6.4 percent of benthic
- sediment samples in the same lake with a concentration ranging from less than 0.41 to 18.8 μ g/kg.
- DCHP was also identified in 13.3 percent of fish tissue (n = 30) with a concentration range from less
- 5612 than 0.22 to 21.9 g/kg (Lee et al., 2019).