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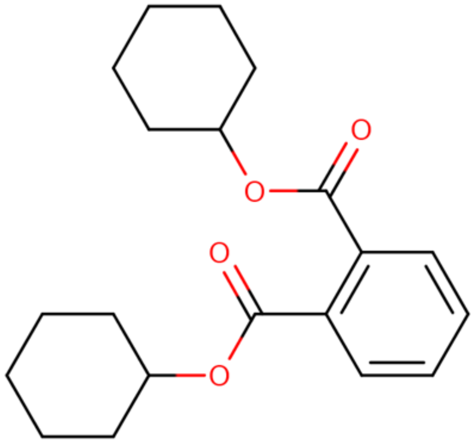
Physical Chemistry and Fate and Transport Assessment for Dicyclohexyl Phthalate (DCHP)

Technical Support Document for the Risk Evaluation

CASRN 84-61-7



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KEY ABBREVIATIONS AND ACRONYMS

CASRN	Chemical Abstracts Service Registry Number
CDR	Chemical Data Reporting
DCHP	Dicyclohexyl phthalate
EC50	Effect concentration at which 50 percent of test organisms exhibit an effect
ECHA	European Chemicals Agency
EPA	Environmental Protection Agency (U.S.)
HLC	Henry’s Law constant
LC50	Lethal concentration at which 50 percent of test organisms die
MDL	Method detection limit
NITE	National Institute of Technology and Evaluation
OCSPP	Office of Chemical Safety and Pollution Prevention (EPA)
OECD	Organisation for Economic Co-operation and Development
OPPT	Office of Pollution Prevention and Toxics (EPA)
QSAR	Quantitative structure-activity relationship
QSPR	Quantitative structure-property relationship
SMILES	Simplified Molecular Input Line Entry System
TRI	Toxics Release Inventory
TSCA	Toxic Substances Control Act
TSD	Technical support document
U.S.	United States
WQP	Water Quality Portal

SUMMARY

This technical support document (TSD) accompanies the Toxic Substances Control Act (TSCA) *Risk Evaluation for Dicyclohexyl Phthalate (DCHP)* (U.S. EPA, 2025d). DCHP is a common chemical name for the chemical substance dicyclohexyl phthalate (CASRN 84-61-7). See Appendix C of the risk evaluation for a complete list of all TSDs and supplemental files included in the DCHP risk evaluation.

DCHP – Chemistry, Fate, and Transport:
Key Points

EPA (or the Agency) evaluated the reasonably available information to characterize DCHP's physical-chemical and environmental fate and transport, the key points of which 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 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), and aerobic or anaerobic biodegradation (Section 3.2.3);
- may be transported through the air and deposited to soil or water (Section 3.4.1);
- will sorb to particulates 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 particulates, 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 likely to biomagnify in aquatic environments (Section 3.6).

EPA considered the reasonably available information identified by the systematic review process under TSCA to characterize the physical chemistry and fate and transport of DCHP. When experimental values were not available, EPI Suite™ 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; and
- will sorb to particulate phases (soil, sediment, air particulate) with a small amount ending up in water when released to all three environmental media/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 $C_{20}H_{26}O_4$ 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. DCHP has a melting point of 66 °C, boiling point of 225 °C (4 mm hg), and Henry's Law coefficient (constant) (HLC) of 9.446×10^{-8} atm-m^3/mol. DCHP has been categorized as a semi-volatile organic compound (SVOC).

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.

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. Review of preliminary 2024 CDR data shows that total production volume for 2023 is similar to the previously reported range. These production volumes suggest that DCHP may have releases from fugitive or stack air emissions, to water, and to landfills during production, distribution, processing in polyvinyl 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 assessment/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.S. EPA, 2021). 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 data set is available in the supplemental file *Risk Evaluation for Dicyclohexyl Phthalate (DCHP) – Systematic Review Supplemental File: Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties* (U.S. EPA, 2025b).

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 *Draft screening assessment: Phthalate substance grouping* (EC/HC, 2017).

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 Suite™ estimated parameters were selected as the representative value for the following physical and chemical parameters: water solubility (WATERNT and WSKOW), K_{OA} (KOAWIN), and HLC (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 Suite™ are provided in Appendix A.

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 (MW)	330.43 g/mol		
Physical form	Solid, prism	(Haynes, 2014)	High
Physical properties	White granular solid	(NLM, 2024)	High
Melting point (MP)	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−07 mmHg	(NLM, 2024)	High
Vapor density	No data		

Property	Selected Value	Reference	Overall Quality Determination
Water solubility	0.030 to 1.48 mg/L [a]	(U.S. EPA, 2017)	Medium
Octanol:water partition coefficient (log K_{OW})	4.82	(EC/HC, 2017)	High
Octanol:air partition ^{c}oefficient (log K_{OA})	10.23 [a]	(U.S. EPA, 2017)	Medium
Henry's Law constant	9.446E−08 atm·m^{3}/mol [a] at 25 °C	(U.S. EPA, 2017)	Medium
Flash point	207 °C	(RSC, 2019)	Medium
Auto-flammability	No data		
Viscosity	Solid, N/A	(NLM, 2024)	High

[a] Modeled value using EPI Suite™

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, and prismatic solid form (NLM, 2024; 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") (U.S. EPA, 2020).

2.4.2 Auto-Flammability

The auto-flammability is the lowest temperature a chemical substance will spontaneously ignite without a spark or flame (Rumble, 2021). Like the flash point, this helps fate assessors to understand the fire hazards of the chemical. 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 Suite™ program is available to model auto-flammability. As such, EPA was not able to model or estimate auto-flammability.

2.4.3 Melting Point

Melting point is one of the inherent properties that informs the chemical's physical state (liquid or solid) at normal environmental conditions. The melting point is the temperature at which a chemical substance coexists as its solid and liquid forms in equilibrium under atmospheric pressure (1 atmosphere) (Rumble, 2021). The physical state information helps assessors understand the environmental fate and transport, as well as the chemical substance's potential exposure routes and bioavailability to both aquatic organisms and humans (occupational and general population). 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, 2024; 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, 2019; 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 study value of 66 °C was selected because it was an experimental primary data point that 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 that often re-reported the Haynes-provided 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 modeled using Epi Suite™ 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 Suite™ were modeled given the limited data availability of DCHP physical chemistry and fate values. The modeled estimate reasonably aligns with the final selected experimental melting point of 66 °C. The EPI Suite™ output is provided in Appendix .

2.4.4 Boiling Point

Boiling point is one of the inherent properties that informs the chemical's physical state (liquid or gas) at normal environmental conditions. The boiling point is the temperature at which a chemical substance coexists in equilibrium as vapor and liquid under atmospheric pressure (Rumble, 2021). The physical state helps inform multiple aspects of the risk evaluation. 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, 2024; Haynes, 2014). Medium-quality sources reported boiling points ranging from 220 to 476.9 °C (RSC, 2019; 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 Suite™ MPBPVP program with a value of 395 °C (U.S. EPA, 2017). All physical chemistry and fate parameters available for modeling using EPI Suite™ were modeled given the limited data availability of DCHP physical chemistry and fate values. The EPI Suite™ output is provided in Appendix A.1.

2.4.5 Density

Density is the chemical substance mass per unit volume (g/mL) (Rumble, 2021) and is one of the inherent properties that informs assessors about the chemical's mobility in the environment under normal conditions. This information assists the assessors in understanding whether the environmental release of DCHP is likely to sink or float in the aquatic systems, or in ambient air. 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/m^3 (NLM, 2024; Haynes, 2014). The three medium-quality sources reported DCHP densities ranging from 0.787 to 1.383 g/m^3 (RSC, 2019; EC/HC, 2015). A density value of 1.383 g/m^3 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

Vapor pressure indicates the pressure exerted by a liquid or solid chemical in equilibrium with its vapor at a given temperature (25 °C for environmental conditions) (40 CFR 796.1950). This information informs the assessors if a chemical substance has the potential to volatilize and be released into the atmosphere, undergo long range transport, and be available for specific exposure pathways. It also helps assessors understand the predicted concentration and environmental releases of a chemical substance to air. A chemical's potential to be present in air is expected to increase as vapor pressure increases. EPA extracted and evaluated six sources containing DCHP vapor pressure information. Three of these sources were excluded as one reported a vapor pressure value collected at 150 °C and the two other sources were identified as duplicates. The remaining three data sources were identified and evaluated as overall high-quality data sources. The overall high-quality sources reported DCHP vapor pressure values ranging from 6.0×10^{-7} to 5.33×10^{-6} mm Hg and a corresponding mean vapor pressure of 2.26×10^{-6} mm Hg (NLM, 2024; Elsevier, 2019; U.S. EPA, 2019; Gobble et al., 2014; Lu, 2009). 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, 2024). This value was selected because it was the closest to the mean of the values reported in the remaining high-quality sources and in close agreement with the estimated vapor pressure value output from the EPI Suite™ 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 Suite™ output is provided in Appendix 4.1.1A.1.

2.4.7 Vapor Density

The vapor density is the mass of a vapor per unit volume of the vapor relative to air (U.S. EPA). The relative vapor density is the ratio between the vapor density of a chemical substance and the vapor density of air (1.0). Relative vapor densities greater than 1 will indicate a higher tendency to sink whereas vapor densities lower than 1 indicate a higher tendency to float in ambient air. This information may inform the fate assessors about the predicted fate and transport of chemical substances (as vapors) when released to ambient air. 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. Because vapor density is not considered a relevant parameter for use in the following fate or exposure assessments and because Epi Suite™ 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

The water solubility indicates the maximum amount of DCHP that will be dissolved in pure water. Water solubility informs many endpoints not only within the realm of fate and transport of DCHP in the environment, but also when modeling for industrial process, and engineering, as well as human and ecological hazard, and exposure assessments. Chemical substances that are soluble in water can be expected to readily disperse through the environment. 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.

The overall high-quality sources reported DCHP water solubility values of 1.01 and 4.00 mg/L (NLM, 2024; 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, 2024; U.S. EPA, 2019; Hollifield, 1979). The value of 1.01 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) whereas the second source reported a water solubility value of 0.35 mg/L estimated by quantitative structure-activity relationship (QSAR) models (Lu, 2009).

Three of the four high-quality sources (NLM, 2024; U.S. EPA, 2019; Hollifield, 1979) and one of the three medium-quality sources (EC/HC, 2017) re-report the (Hollifield, 1979) 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). Furthermore, the Hollifield study employed a rapid nephelometric technique intended to replace slower, more sophisticated measurement methodologies of the time. The study discusses the nephelometric technique employed, citing inherent limitations due to the use of a co-solvent, and difficulty in achieving a stable turbid solution over the time intervals sampled to attain accurate measurements. Occurrence of unstable solutions over the sampling intervals may lead to an inaccurate standard curve from which the solubility of DCHP was ultimately extrapolated from. The standard samples used to create the curve were created utilizing “practical grade” DCHP, as opposed to samples prepared using a 99 percent purity chemical solution for other chemicals in the study. This “practical grade” mixture, along with the nephelometric technique and tendency of DCHP to form colloidal suspensions while in solution, resulted in less precise results for DCHP of ±20 percent in the study (Hollifield, 1979). While perhaps a viable method of estimating an accurate water solubility for DCHP in1979 when the study was conducted, the Hollifield study is an extrapolated/modeled value and is not equivilent to OECD 105 standard experimental water solubility guideline test, or other equivalent measurements, and should not be considered of equal quality and reliability.

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 Suite™ programs to characterize the range of uncertainty associated with the DCHP solubility based on a variety of physical and chemical parameters. EPI Suite™ is a standard QSAR tool used by EPA to assess chemicals under TSCA.

Within EPI Suite™ EPA used two different programs to estimate DCHP water solubility. EPI Suite™ 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 Simplified Molecular Input Line Entry System (SMILES) and a combination of user-input (EPA-selected) or EPI Suite™-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 Suite™ estimated K_{OW} (6.20) and MW (330.43 g/mol) values,
   b. SMILES code with EPI Suite™ estimated K_{OW} (6.20) and EPA selected MP (66 °C),

   c. SMILES code with EPI Suite™ 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

ID	Model	K_{OW}	MP (°C)	MW (g/mol)	Solubility (mg/L)
1a	WSKOWWIN	6.20[a]	N/A[b]	330.43[b]	0.041
1b	WSKOWWIN	6.20[a]	66[c]	N/A	0.0696
1c	WSKOWWIN	4.82[b]	N/A[b]	330.43[b]	0.621
1d	WSKOWWIN	4.82[b]	66[c]	N/A	1.48
2	WATERNT	N/A	N/A	N/A	2.40

SMILES: C1CCC(CC1)OC(=O)c2ccccc2C(=O)OC3CCCCC3
[a] Estimated from Epi Suite™ KOWWIN
[b] MW used when user-entered MP is not available
[c] EPA-selected value

A maximum water solubility value of 1.48 mg/L was calculated via EPI Suite's™ WSKOWWIN estimation program with a known experimentally determined K_{OW} (4.82) and melting point (66 °C). For phthalates, EPI Suite™ 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 water solubility value of 1.01 mg/L reported by EC/HC is based on EPI Suite™ estimate that used an estimated K_{OW} (6.20). A water solubility value of 2.40 mg/L was estimated using the EPI Suite™ WATERNT estimation program. The EPI Suite™ output is provided in Appendix A.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 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). Althoug the toxicology study was not explicitly a water solubility study, the source material is considered high in quality by EPA and was the sole study that reported empirical data pertaining to DCHP at lower concentrations ranges. The observed value lower-range value aligns reasonably with the EPI Suite™ 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 Suite™ SKOWWIN output values (Appendix A.2.2). The value reasonably aligns with the uppermost perceived water solubility value of 1.01 mg/L collected experimentally via OECD 105 as stated by

EC/HC (EC/HC, 2017). The EPI Suite™ 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 Suite™ 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 (1.01 mg/L) (EC/HC, 2017). The true solubility of DCHP can be lower than the 1.48 mg/L, with concentrations in the environment expected to be lower based on environmental monitoring data (Keil et al., 2011).

2.4.9 Octanol-Water Partitioning Coefficient

The octanol-water partition coefficient (K_{OW}) provides information on how the chemical, under equilibrium, will partition between octanol (which represents the lipids or fats in biota) and water (U.S. EPA, 2025). This informs on how the chemical is likely to partition in the environment as well as for the estimation of other properties including water solubility, bioconcentration, soil adsorption, and aquatic toxicity. 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 high-quality with a reported log K_{OW} value of 4.82 (EC/HC, 2017). Three of the sources were determined to be 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, 2019; Cao, 2010; Lu, 2009). One source was determined to be of low quality with a reported log K_{OW} value of 5.6 (NCBI, 2020). A value of 4.82 was selected as the representative log K_{OW} value for DCHP with a high overall confidence determination (EC/HC, 2017). The 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 Suite™ output is provided in Appendix 4.1.1A.3.

2.4.10 Octanol-Air Partitioning Coefficient

The octanol-air partition coefficient (K_{OA}) provides information on how the chemical, under equilibrium, will partition between octanol and air (U.S. EPA, 2025). This informs fate assessors on how the chemical is likely to partition in the environment between air and aerosol particles, air and foliage, and air and soil. This information also helps to understand how chemical substances are expected to behave in the atmosphere and in human respiratory tissues. Chemical substances with high K_{OA} are more likely to sorb onto solid surfaces as well as to bioaccumulate in the human respiratory tissue. EPA extracted and evaluated data from a single source containing information regarding DCHP octanol-air 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 Suite™ (U.S. EPA, 2017). The EPI Suite™ 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 Suite™ derived value of 10.23 as the representative log K_{OA} value for use in risk assessment (U.S. EPA, 2017). The EPI Suite™ 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 that 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 Suite™ output is provided in Appendix A.4.

2.4.11 Henry's Law Constant

The Henry's Law constant (HLC) of a chemical substance is the ratio of the substance's vapor pressure and water solubility (U.S. EPA, 2025). The HLC (atm×m^3/mol) provides an indication of a chemical's volatility from water and gives an indication of potential environmental partitioning, potential removal in sewage treatment plants during air stripping, and possible routes of environmental exposure. No data were available in the literature surveyed during systematic review pertaining to the HLC for DCHP. EPA estimated a representative HLC of 9.446×10^{-8} atm·m^3/mol at 25 °C via EPI Suite™ for use as the representative k_h value for DCHP (U.S. EPA, 2017) because no other empirical or modeled values were available. The estimated value is in close agreement with the HLC of 1.01×10^{-7} atm·m^3/mol in the experimental values reported within the EPI Suite™ KOHWIN database (U.S. EPA, 2017). EPA selected the HLC of 9.446×10^{-8} atm·m^3/mol at 25 °C for use in risk assessment of DCHP. The EPI Suite™ 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 air-water 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 (Lu, 2009). Two log K_{AW} values, −4.52 (bond estimate and −5.58 (group estimate), were calculated from the HLC (k_h) estimated from the EPI Suite™ HENRYWIN program (T = 289.15 K, R = 8.205×10^{-5} atm-m^3/mol-K) (U.S. EPA, 2017). EPA has selected the QSPR-derived value of −3.56 for use as the representative K_{AW} (Lu, 2009). 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 Suite™ estimated value since EPI Suite™ currently does not have a program that can directly estimate air-water partitioning values. Instead, the EPI Suite™ value must be back-calculated indirectly using the HLC estimated from Epi Suite's™ HENRYWIN™ program. The EPI Suite™ output is provided in Appendix A.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 (Lu, 2009). 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 Suite™ estimates, which range from 3.46 to 4.22 (U.S. EPA, 2017). Lacking adequate experimental data to validate modeled values, EPA has overall medium quality determination in the selected QSPR-derived K_{OC} value. The EPI Suite™ output is provided in Appendix A.6.

2.4.14 Flashpoint

The flash point is the lowest temperature at which a substance produces sufficient vapor to form an ignitable mixture with air (U.S. EPA, 2025). This helps fate assessors understand the fire hazards of the chemical. 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, 2019). Epi Suite™ does not offer a modeling program with the capacity to estimate chemical flashpoint.

As such, flash point was not estimated using Epi Suite™. The Agency selected a flash point of 207 °C because of the lack of high-quality data (RSC, 2019). The selected value is consistent with the value selected in the final scope for DCHP (U.S. EPA, 2020).

2.4.15 Viscosity

Viscosity is the expected flow resistance of a chemical substance due to molecular friction within a fluid (U.S. EPA, 2025). This helps fate assessors to understand the transport of a chemical substance directly released to the environment. 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, 2024). 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, 2024). 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 Suite™ 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 Suite™ 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 Suite™ 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 fully extracted dataset is available in the supplemental file *Risk Evaluation for Dicyclohexyl Phthalate (DCHP) – Systematic Review of Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport* (U.S. EPA, 2025a).

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

Table 3-1. EPI Suite™ Input Values

Property	Input Value	Reference
Chemical name	Dicyclohexyl phthalate	–
SMILES	C1CCC(CC1)OC(=O)C2=CC=CC=C2C(=O)OC3CCCCC3	–
Melting point	66 °C	(Haynes, 2014)
Vapor pressure	8.69E−07 mmHg	(NLM, 2024)
Water solubility	≤1.48 mg/L	(U.S. EPA, 2017)
Log K_{OW}	4.82	(EC/HC, 2017)

Several fate parameters were modeled using EPA Epi Suite™ 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 Suite™ HYDROWIN program was used to estimate the hydrolytic half-life at a pH of 7 and 8 at 25 °C. The EPI Suite™ 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). Although 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 can promote DCHP 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 distribution systems following drinking water treatment. In systems with a pH value exceeding 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 DCHP by hydrolysis.

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 Suite™ was used to estimate the atmospheric oxidation half-life of DCHP at 0.441 days (5.288 hours), indicating that atmospheric oxidation can 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.

While photolysis can 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 of DCHP 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 to 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 can 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 biodegradation in water	8.1 (91% in 28 days, pseudo-first order)	Not reported	(EC/HC, 2015)	Medium
	16.8 (68.5% in 28 days, pseudo-first order)	Not reported	(NCBI, 2020)	Medium
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

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 can favor one media over another. Empirical values were included when available. Estimated values from QSPR models (obtained from literature) and EPI Suite™ 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 (K_{OW})	6.07E04	4.82	(EC/HC, 2017)	Organic carbon
	1.59E06	6.2026 (KOWWIN™)[b]	(U.S. EPA, 2017)	Organic carbon
Organic Carbon:Water (K_{OC})	2.95E04 L/kg	4.47 (QSPR)	(Lu, 2009)	Organic carbon
	1.66E04 L/kg	4.22 (KOCWIN™)[b]	(U.S. EPA, 2017)	Organic carbon
Octanol:Air (K_{OA})	1.58E09	9.20 (QSPR)	(Lu, 2009)	Organic carbon

Parameter	Value[a]	Log Value[a]	Reference	Predominant Phase
	1.70E10	10.23 (KOAWIN™)[b]	(U.S. EPA, 2017)	Organic carbon
Air:Water (K_{AW})	3.63E−03	−3.56 (QSPR)	(Lu, 2009)	Water
	3.01E−05	−4.52 (Bond Estimate, HENRYWIN™)[b]	(U.S. EPA, 2017)	Water
	2.63E−06	−5.58[c] (Group Estimate, HENRYWIN™)	(U.S. EPA, 2017)	Water

[a] Measured unless otherwise noted.

[b] Information was estimated using EPI Suite™ (U.S. EPA, 2017); 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−08 atm·m^3/mole, SMILES: O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2`

[c] Calculated using the relationship HLC = R×T×K_{AW} where R is the universal gas constant equal to 8.206E−05 atm·m^3/mol·K

The value of the partitioning coefficients in Table 3-3 suggest that DCHP will most likely exist primarily sorbed to particulate matter. Although 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 Suite™ estimated values with a clear preference to exist in particulates (organic carbon, sediment, soil, air particulates, and dust) over the water and air compartments. While 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, 2024). 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 Suite™ estimates that a smaller fraction of DCHP could be sorbed to airborne particulates and these particulates can be resistant to atmospheric oxidation. DCHP can be deposited in surface waters or to the surface of soil through direct deposition of atmospheric particulates 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 can 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 air-water partitioning, and HLC 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 particulates in water or to sediment particulates with a K_{OW} and K_{OC} exceeding 1.

In particulates and sediment, DCHP is likely to be shielded from sunlight and unable to undergo abiotic transformation by photolysis but can 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 can 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.

DCHP can 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 previous 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 Suite™ Tier III Fugacity outputs are provided in Appendix A.8.

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

Release Scenario	Release Rate (kg/hr)	Air (%)	Water (%)	Soil (%)	Sediment (%)
Equal Release	1,000	0.2	13.2	**76.4**	10.2
100% Air Release	1,000	1.4	2.4	**94.3**	1.85
100% Soil Release	1,000	<0.01	0.05	**99.9**	0.04
100% Water Release	1,000	<0.01	**56.5**	0.04	43.5

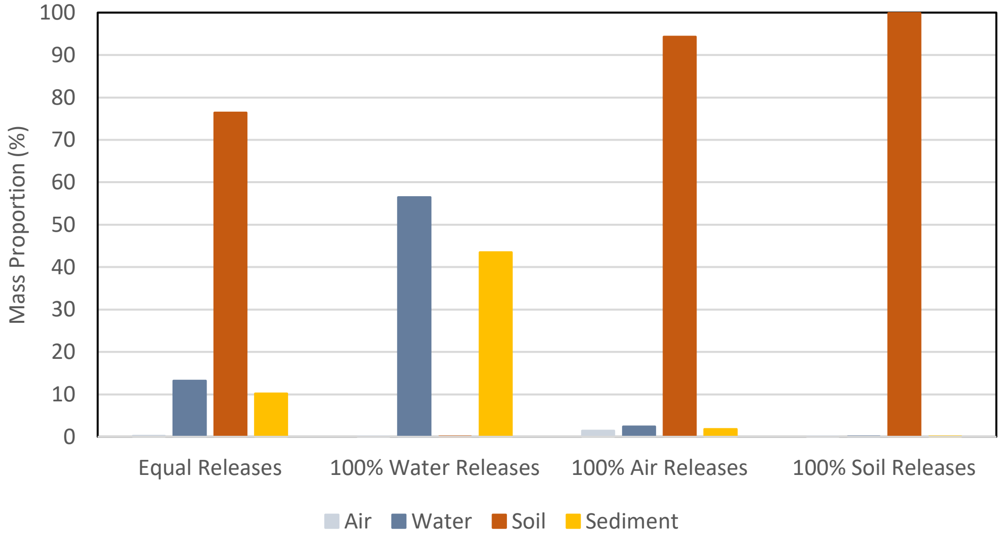

Figure 3-1. EPI Suite™ Level III Fugacity Model Graphical Summary

DCHP can 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 can be scavenged by precipitation. The fraction of DCHP that 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 can 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 and can be biologically degraded aerobically or anaerobically in tandem with abiotic processes. DCHP is also likely to partition to suspended and benthic sediments from surface water that can 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 can 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 can degrade biologically under aerobic or anaerobic conditions as well as by hydrolysis and is not expected to be persistent.

DCHP can be introduced to soil by deposition from the atmosphere or through precipitation. It can 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 particulates 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.

In wastewater, DCHP has been observed to be removed primarily through sorption to organic material and removal via sludge. Some minor removal can 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 considered a significant transport pathway.

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

3.4 Media Assessments

3.4.1 Air and Atmosphere

As described in the *Environmental Release and Occupational Exposure Assessment for Dicyclohexyl Phthalate (DCHP)* (U.S. EPA, 2025c), 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 can sorb to particulates or solidify, settling out of the air. DCHP can be present in particulates 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. Photo-oxidation occurs on the surface of air particulates. 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 HLC and octanol-air partitioning coefficient (K_{OA}). Photo-oxidization can also be limited because of competing sorption processes. The EPI Suite™ AEROWIN™ model predicts that 25.1 to 44.9 percent of atmospheric DCHP can 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 can be shielded from direct sunlight. While it can degrade rapidly due to photo-oxidation, some medium-to-long transport of DCHP is still possible. DCHP in the atmosphere can be deposited into surface water bodies or soil with a measured flux of 0.088 to 0.433 µg/m^2-day (Zeng et al., 2010). Precipitation (*e.g.*, rain) can 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

Although several studies examine the concentration of DCHP in indoor air particulates and dust, only two were conducted within the United States. The U.S. studies are summarized below and the international monitoring studies are provided in Appendix B.1. The foreign studies are not discussed further because it is unclear how environmental factors contributing to DCHP media concentrations may vary nationally and internationally. 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 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. The study authors reported 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 particulates 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 because it is unclear how environmental factors contributing to DCHP media concentrations may vary between the United States and other countries. However, these studies do support that DCHP can be found in air particulates 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 *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.S. EPA, 2025c). It is possible for DCHP to reach surface water through atmospheric deposition, precipitation, and through wastewater treatment plant discharges (Wu et al., 2019; Peters et al., 2008). If DCHP enters surface water, it is expected to partition to suspended organic material present in the water column and sediment (Section 3.3). Although information about the presence of DCHP in U.S. wastewater treatment facilities is very limited, DCHP has been extracted and quantified in wastewater treatment plant particulate material and biosolids in China (Wu et al., 2019; Zhu et al., 2019; Meng et al., 2014). Sorption and biological treatment processes were reported to play the primary role in removing DCHP from wastewater with overall DCHP removal efficiencies of 68.60 to 97.97 percent (Wu et al., 2019).

There are very limited monitoring data for DCHP in surface waters reported to monitoring databases such as the Water Quality Portal (WQP) that 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 seawater samples with column concentrations of up to 15 ng/L DCHP in Puget Sound, Washington, and Barkley Sound in British Columbia, Canada (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. Although international studies do support the idea that DCHP may be present in surface water and suspended particulates, the specific values may not be a viable direct comparison to the United States. For this reason, details of the international studies extracted during systematic review are not included in this section but are reported in Appendix B.3.

DCHP is susceptible to hydrolysis (Section 3.2.1) to form monocyclohexyl phthalate and cyclohexanol via acid ester hydrolysis with an estimated half-life of 426 days at pH of 8 and 25 °C. 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. Although atmospheric oxidation (indirect photolysis) was estimated using EPI Suite™ (Section 3.2.2), it is unclear if the estimated atmospheric transformation degradation rate would translate to aquatic environments. It is likely that photolysis can 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 can persist for days to weeks. However, binding to sediment reduces the bioavailability of DCHP in soils and sediments that can increase the persistence.

3.4.2.2 Sediments

DCHP can exist in sediments following releases to surface waters as described in the release assessments (U.S. EPA, 2025c). Once in water, the EPI Suite™ level III Fugacity Model suggests that up to 43.5 percent of total DCHP mass can 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. Although 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 WQP 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 with concentrations of 66.5 and 73.7 µg/kg. Reporting limits for the Washington state monitoring program varied widely, ranging from 30.1 to 93 µg/kg.

Based on the water solubility (≤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 can be less bioavailable for degradation and therefore 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 can act as a long-term reservoir and source to contaminated water bodies. However, once in sediments, DCHP is expected to biodegrade in the order of days to weeks with reported half-lives of 11.1 days and 26.4 days in sediments under aerobic and anaerobic conditions, respectively (Yuan et al., 2002).

3.4.3 Terrestrial Environments

3.4.3.1 Soil

DCHP may be present in soil through various means including dry and wet deposition and field application of biosolids. DCHP has been observed to deposit directly from the atmosphere to soil (Zeng et al., 2010; Vethaak et al., 2005). These studies reported the presence of DCHP in rainwater and air samples collected from the Netherlands and China, respectively. In the Netherlands DCHP was detected in rainwater samples collected near the North Sea Canal at concentrations below 8 ng/L (Vethaak et al., 2005). Air samples collected in China reported higher DCHP deposition flux in areas near industrial and anthropogenic activities (Zeng et al., 2010). The study reported DCHP median deposition air fluxes of

0.236, 0.0.84, and 0.029 µg/m^2-d in urban areas with high industrial use of plastics, urban residential areas, and suburban areas with limited anthropogenic activities. Although no TRI data has reported the field application of biosolids, DCHP has been shown to exist in wastewater sludge and final biosolids samples collected from municipal WWTPs in China at concentrations ranging from 9.3 ng/g-dw sludge to 310 ng/g-dw sludge 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 Suite™ 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 can also partition to soil when released to other environmental compartments; EPI Suite™ estimated 76.4 of DCHP released to air can 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 via atmospheric deposition. DCHP has a Henry's law constant of 9.446×10^{-8} atm·m^3/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 indicating the occurrence of DCHP in soils within the United States. Five studies reported the presence of DCHP in China. Although these studies demonstrate that DCHP can be present in soil, it is unlikely that the international studies are appropriate for a direct comparison to U.S. 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 to 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 particulates and organic media (log $K_{OW} = 4.82$; log $K_{OC} = 4.47$) and low water solubility (≤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, because the data may not accurately reflect the concentrations of DCHP in American wastewater treatment systems, they 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 particulates, 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). DCHP 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

In this assessment/TSD, landfills were divided into two zones: (1) an "upper-landfill" zone with normal environmental temperatures and pressures, where biotic processes are the predominant route of degradation for DCHP; and (2) 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 can 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 can be as high as 70 °C, biotic processes are significantly inhibited and are likely to be completely irrelevant at temperatures above 60 °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 can 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 can 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 particulates and organic media (log K_{OW} = 4.82; log K_{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 that can 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.

Due to DCHP's high potential to sorb to organic media it is assumed that 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.

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/; accessed November 24, 2025); 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 slower rates of 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 Suite™ (LEV3Epi) (Appendix A.10), DCHP's overall environmental half-life was estimated to be approximately 64 days (U.S. EPA, 2017). Therefore, while 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 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 to 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 (Kickham et al., 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, which 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).

While EPA does have information from laboratory studies that provide evidence of and rates of biodegradation of DCHP in aerobic environments, biodegradation is not the primary removal mechanisms of DCHP in wastewater treatment processes. The hydraulic retention time of the standard WWTP in the United States is about 18 hours. The biodegradation half-life of DCHP is measured in days to weeks in saturated sediment and water (NCBI, 2020; EC/HC, 2015; Yuan et al., 2002). Sorption to sludge is the primary method of removal of DCHP in wastewater treatment processes.

STPWIN™, an EPI Suite™ 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 accounted 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 partial 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 was 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 whereas landfills are discussed in Section 3.4.3.3.

EPI Suite™ 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 (≤1.48 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 Suite™ (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; accessed November 24, 2025), 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 (≤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 Suite™, which predicts a log BCF of 2.85 and log BAF of 1.83 for DCHP (U.S. EPA, 2017).

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, Arizona. Twenty-one fish were sampled from 11 fisheries within metro-Phoenix. Although phthalates were found in all 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 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 Suite™ 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 particulates in the air or be deposited into adjacent water bodies and soil. DCHP can 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 can all be minor pathways for short-range transport. However, DCHP in water is expected to partition out of the water phase and adsorb to particulates 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 through 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 HLC.

Biodegradation would be further hindered in anoxic or anaerobic conditions, such as 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 Suite™ 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.

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

- can degrade to monocyclohexyl phthalate and cyclohexanol (Sections 3.2.1, 3.2.2, and 3.2.3);
- will not significantly degrade via hydrolysis (Section 3.2.1) under standard environmental conditions;
- can 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);
- can be susceptible to long-range transport and deposition to water and soil via the atmosphere (Section 3.4.1);
- will partition to organic particulates in indoor and outdoor air (Sections 3.4.1.1 and 3.4.1.2); and
- will partition to organic particulates 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);
- 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 not likely to be bioaccumulative (Section 3.6).

Findings that were found to have a robust weight of evidence supporting them had one or more high-quality 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

Appendix A EPI SUITE™ MODEL OUTPUT

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

Run Date: 2024-06-12.

```
Experimental Database Structure Match:
  Name     :  DICYCLOHEXYL PHTHALATE
  CAS Num  :  000084-61-7
  Exp MP (deg C):  66
  Exp BP (deg C):  224 @ 4 mm Hg
  Exp VP (mm Hg):  8.69E-07  (extrapolated)
         (Pa   ):  1.16E-004
  Exp VP (deg C):  25
  Exp VP ref    :  WERNER,AC (1952)

SMILES : C1CCC(CC1)OC(=O)c2ccccc2C(=O)OC3CCCCC3
CHEM   : Dicyclohexyl Phthalate
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: 394.85 deg C (estimated))
  (Using MP: 66.00 deg C (exp database))
    VP:  1.07E-006 mm Hg (Antoine Method)
      :  0.000142 Pa  (Antoine Method)
    VP:  4.58E-006 mm Hg (Modified Grain Method)
      :  0.00061 Pa  (Modified Grain Method)
    VP:  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)
  Subcooled liquid VP:  2.21E-006 mm Hg (25 deg C, exp database VP )
                     :  0.000295 Pa  (25 deg C, exp database VP )

-------+-----+--------------------+----------+---------
 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
============+====================+==========+=========
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
-------------------------------------------------------
```

```
-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group | 10  |  -CH2- (ring)      |    7.75  |   77.50
 Group |  2  |  >CH-  (ring)      |   19.88  |   39.76
 Group |  2  |  -COO- (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
-------------------------------------------------------

------------------------------------------------------------------------------
```

A.2 Water Solubility

Two separate EPI Suite™ 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.

```
                  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 : C1CCC(CC1)OC(=O)c2ccccc2C(=O)OC3CCCCC3
CHEM   : Dicyclohexyl Phthalate
MOL FOR: C20 H26 O4
MOL WT : 330.43
---------------------------------- WSKOW v1.43 Results -------------------------
Log Kow  (estimated)  :  6.20
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  4.82 (user entered)

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 deg C (Use Tm = 25 for all liquids)

      Correction(s):         Value
      --------------------   -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -5.349
   Water Solubility at 25 deg C (mg/L):  1.48

------------------------------------------------------------------------------
```

A.2.2 Water Solubility (WATERNT)

Run Date: 2024-06-12.

```
                  Water Sol (v1.01 est): 2.4027 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 : C1CCC(CC1)OC(=O)c2ccccc2C(=O)OC3CCCCC3
CHEM   : Dicyclohexyl Phthalate
MOL FOR: C20 H26 O4
MOL WT : 330.43
-------+-----+--------------------------------------------+----------+---------
 TYPE  | NUM |    WATER SOLUBILITY FRAGMENT DESCRIPTION   |  COEFF   |  VALUE
-------+-----+--------------------------------------------+----------+---------
 Frag  |  2  |  -CH      [aliphatic carbon]               |-0.5285   | -1.0570
 Frag  |  4  |  Aromatic Carbon  (C-H type)               |-0.3359   | -1.3435
 Frag  |  2  |  -C(=O)O  [ester, aromatic attach]         | 0.7006   |  1.4012
 Frag  |  2  |  Aromatic Carbon  (C-substituent type)     |-0.5400   | -1.0799
 Frag  | 10  |  -CH2-  [aliphatic carbon, cyclic]         |-0.3308   | -3.3084
 Const |     |  Equation Constant                         |          |  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(=O)c2ccccc2C(=O)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(=O)O  [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(=O)c2ccccc2C(=O)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)
 Henry LC: 7.39e-007 atm-m3/mole (HenryWin bond estimate)

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

-----------------------------------------------------------------------------
```

A.5 Henry's Log (HENRYWIN)

Run Date: 2024-06-12.

```
       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 : C1CCC(CC1)OC(=O)c2ccccc2C(=O)OC3CCCCC3
CHEM   : Dicyclohexyl Phthalate
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
----------+---------------------------------------------+---------+----------
   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
----------+---------------------------------------------+---------+----------
 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)                     |            | -1.50
         |             2  CH (C)(C)(O)                   |            |  0.24
         |             4  Car-H (Car)(Car)               |            |  0.44
         |             2  Car (Car)(Car)(CO)             |            | -1.68
         |             2  CO (O)(Car)                    |            |  9.14
         |             2  O (C)(CO)                      |            | -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
-----------------------------------------------------------------------------
```

A.6 K_{OC} (KOCWIN)

Run Date: 2024-06-12.

```
SMILES : C1CCC(CC1)OC(=O)c2ccccc2C(=O)OC3CCCCC3
CHEM   : Dicyclohexyl Phthalate
MOL FOR: C20 H26 O4
MOL WT : 330.43
---------------------------  KOCWIN v2.01 Results  ---------------------------
```

```
  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):
                  2   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   )  ......................... :  4.82
         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   <===========


------------------------------------------------------------------------------
```

A.7 Hydrolysis Degradation Rate (HYDROWIN)

Run Date: 2024-06-18

```
SMILES : C1CCC(CC1)OC(=O)c2ccccc2C(=O)OC3CCCCC3
CHEM   : Dicyclohexyl Phthalate
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 "**".

ESTER:  R1-C(=O)-O-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(=O)-O-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™ Fugacity Tier III model was run for four scenarios: 1000 kg/hr release to air, 1000 kg/hr release to water, 1000 kg/hr release to soil, 1000 kg/hr release to all compartments (air, water, soil).

A.8.1 Release to Air

Run Date: 2024-06-21

```
CAS Number: 000084-61-7
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)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(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
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(=O)O  [ester, aromatic attach]         |-0.7121   | -1.4242
 Const |     |  Equation Constant                         |          |  0.2290
-------+-----+--------------------------------------------+----------+--------
                                                             Log Kow   =   6.2026


MPBPVP (v1.43) Program Results:
===============================
Experimental Database Structure Match:
  Name     :  DICYCLOHEXYL PHTHALATE
  CAS Num  :  000084-61-7
  Exp MP (deg C):  66
  Exp BP (deg C):  224 @ 4 mm Hg
  Exp VP (mm Hg):  8.69E-07  (extrapolated)
         (Pa   ):  1.16E-004
  Exp VP (deg C):  25
  Exp VP ref    :  WERNER,AC (1952)

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)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)
      :  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)
  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 |  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
============+====================+==========+=========
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
------------------------------------------------------

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group | 10  |  -CH2- (ring)      |    7.75  |   77.50
 Group |  2  |  >CH-  (ring)      |   19.88  |   39.76
 Group |  2  |  -COO- (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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
---------------------------------- WSKOW v1.43 Results ------------------------
Log Kow  (estimated)  :  6.20
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  4.82 (user entered)

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 deg C (Use Tm = 25 for all liquids)

      Correction(s):        Value
      --------------------   -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -5.349
   Water Solubility at 25 deg C (mg/L):  1.48
```

```
WATERNT Program (v1.01) Results:
===============================

                  Water Sol (v1.01 est): 2.4027 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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
-------+-----+--------------------------------------------+----------+---------
 TYPE  | NUM |    WATER SOLUBILITY FRAGMENT DESCRIPTION   |  COEFF   |  VALUE
-------+-----+--------------------------------------------+----------+---------
 Frag  |  2  |  -CH      [aliphatic carbon]               |-0.5285   | -1.0570
 Frag  |  4  |  Aromatic Carbon  (C-H type)               |-0.3359   | -1.3435
 Frag  |  2  |  -C(=O)O  [ester, aromatic attach]         | 0.7006   |  1.4012
 Frag  |  2  |  Aromatic Carbon  (C-substituent type)     |-0.5400   | -1.0799
 Frag  | 10  |  -CH2-  [aliphatic carbon, cyclic]         |-0.3308   | -3.3084
 Const |     |  Equation Constant                         |          |  0.2492
-------+-----+--------------------------------------------+----------+---------
                              Log Water Sol (moles/L) at 25 dec C  =   -5.1384
                              Water Solubility (mg/L) at 25 dec C  =   2.4027


ECOSAR Program (v1.11) Results:
===============================
ECOSAR Version 1.11 Results Page

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
CAS Num:
ChemID1:
MOL FOR: C20 H26 O4
MOL WT : 330.43
Log Kow: 6.203      (EpiSuite Kowwin v1.68 Estimate)
Log Kow:            (User Entered)
Log Kow:            (PhysProp DB exp value - for comparison only)
Melt Pt: 66.00      (deg C, User Entered for Wat Sol estimate)
Melt Pt: 66.00      (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 0.06964    (mg/L, EpiSuite WSKowwin v1.43 Estimate)
Wat Sol: 1.48       (mg/L, User Entered)
Wat Sol: 4          (mg/L, PhysProp DB exp value)


--------------------------------------
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
                                                                    Predicted
ECOSAR Class                 Organism            Duration  End Pt    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)                     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)


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

----------+---------------------------------------------+---------+----------
   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
----------+---------------------------------------------+---------+----------
 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)                      |           | -1.50
        |           2  CH (C)(C)(O)                    |           |  0.24
        |           4  Car-H (Car)(Car)                |           |  0.44
        |           2  Car (Car)(Car)(CO)              |           | -1.68
        |           2  CO (O)(Car)                     |           |  9.14
        |           2  O (C)(CO)                       |           | -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:
======================================

          Log Koa: 10.233

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
--------------------------- KOAWIN v1.10 Results -------------------------

Log Koa (octanol/air) estimate:  10.233
    Koa (octanol/air) estimate:  1.711e+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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 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
   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(=O)-O-C]                      |  0.1742 |  0.3484
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.1573
 Const|  *  |  Equation Constant                         |         |  0.7475
============+============================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)     |         |  0.9386
============+============================================+=========+=========

------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin2 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-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
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-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(=O)-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        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  0.2319 |  0.4638
 Frag |  4  |  Aromatic-H                                |  0.0004 |  0.0016
 Frag | 10  |  -CH2-  [cyclic]                           |  0.0141 |  0.1411
 Frag |  2  |  -CH -  [cyclic]                           |  0.0079 |  0.0158
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.5211
 Const|  *  |  Equation Constant                         |         |  0.5544
============+============================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)  |         |  0.6556
============+============================================+=========+=========
------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin6 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
```

```
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  1.5833 |  3.1665
 Frag |  4  |  Aromatic-H                                |  0.0342 |  0.1368
 Frag | 10  |  -CH2-  [cyclic]                           |  0.1206 |  1.2058
 Frag |  2  |  -CH -  [cyclic]                           |  0.0294 |  0.0589
 MolWt|  *  |  Molecular Weight Parameter                |         | -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


------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin7 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  0.1719 |  0.3437
 Frag |  4  |  Aromatic-H                                | -0.0954 | -0.3817
 Frag | 10  |  -CH2-  [cyclic]                           | -0.1200 | -1.2001
 Frag |  2  |  -CH -  [cyclic]                           |  0.0395 |  0.0789
 Const|  *  |  Equation Constant                         |         |  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
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.


BioHCwin (v1.01) Program Results:
==============================
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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)):
       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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   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


KOCWIN Program (v2.00) Results:
==============================
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
--------------------------  KOCWIN v2.01 Results  --------------------------

  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):
                  2   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   )  ......................... :  4.82
         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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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 "**".

ESTER:  R1-C(=O)-O-R2                ** R1: -Phenyl
                                        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(=O)-O-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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 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:
===========================================================
------+-----+---------------------------------------------+---------+---------
 TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION  |  COEFF  |  VALUE
------+-----+---------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                       | -0.7605 | -1.5211
 Frag |  4  |  Aromatic-H                                 |  0.2664 |  1.0655
 Frag | 10  |  -CH2-  [cyclic]                            |  0.0963 |  0.9625
 Frag |  2  |  -CH -  [cyclic]                            |  0.0126 |  0.0252
 Frag |  1  |  Benzene                                    | -0.4277 | -0.4277
 L Kow|  *  |  Log Kow =   4.82 (user-entered   )         |  0.3073 |  1.4814
 MolWt|  *  |  Molecular Weight Parameter                 |         | -0.8473
 Const|  *  |  Equation Constant                          |         | -1.5371
============+=============================================+=========+=========
   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   |
============+=============================================+=========+=========

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)

                             RIVER             LAKE
                           ---------         ---------
Water Depth     (meters):   1                 1
Wind Velocity    (m/sec):   5                 0.5
Current Velocity (m/sec):   1                 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
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
          -Aeration tank       0.00      9635.43       10000.00
          -Settling tank       0.00      9635.43       10000.00

 STP Overall Chemical Mass Balance:
 ---------------------------------
                             g/h               mol/h          percent

Influent                    1.00E+001         3.0E-002        100.00

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

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 (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
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       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+000          1.2E-002        38.51
Waste sludge                2.37E-001          7.2E-004         2.37
Primary volatilization      1.25E-005          3.8E-008         0.00
Settling volatilization     3.02E-006          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
Settling biodegradation     3.10E-001          9.4E-004         3.10
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+000          2.9E-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)
  Melting Pt  : 66 deg C (user-entered)
  Log Kow     : 4.82  (user-entered)
  Soil Koc    : 1.33e+004  (KOCWIN MCI method)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       1.43            10.6         1000
   Water     2.41            900          0
   Soil      94.3            1.8e+003     0
   Sediment  1.85            8.1e+003     0
```

```
             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       5.05e-012    630         96.1        63          9.61
   Water     2.26e-014    12.5        16.2        1.25        1.62
   Soil      3.15e-014    244         0           24.4        0
   Sediment  2.78e-014    1.07        0.249       0.107       0.0249

   Persistence Time: 672 hr
   Reaction Time:    757 hr
   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)
   Air       1.43            10.6          1000
   Water     2.41            900          0
     water     (2.35)
     biota     (0.00778)
     suspended sediment (0.047)
   Soil      94.3            1.8e+003     0
   Sediment  1.85            8.1e+003     0

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      10.58
      Water:    900
      Soil:     1800
      Sediment: 8100
        Biowin estimate: 2.749  (weeks-months)

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004


Level III Fugacity Model (Full-Output): EQC Default
=====================================================
  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)
  Melting Pt  : 66 deg C (user-entered)
  Log Kow     : 4.82  (user-entered)
  Soil Koc    : 2.71e+004  (EQC Model Default)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       1.41            10.6          1000
   Water     2.25            900          0
   Soil      92.9            1.8e+003     0
   Sediment  3.47            8.1e+003     0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       5.05e-012    630         96.1        63          9.61
   Water     2.11e-014    11.8        15.4        1.18        1.54
   Soil      1.55e-014    244         0           24.4        0
   Sediment  2.6e-014     2.03        0.474       0.203       0.0474

   Persistence Time: 683 hr
   Reaction Time:    769 hr
   Advection Time:   6.1e+003 hr
   Percent Reacted:  88.8
   Percent Advected: 11.2
```

```
  Water Compartment Percents:
 --------------------------
        Mass Amount    Half-Life    Emissions
         (percent)        (hr)       (kg/hr)
 Air       1.41           10.6         1000
 Water     2.25           900          0
   water     (2.16)
   biota     (0.00712)
   suspended sediment (0.0876)
 Soil      92.9           1.8e+003     0
 Sediment  3.47           8.1e+003     0

 Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
    Air:      10.58
    Water:    900
    Soil:     1800
    Sediment: 8100
      Biowin estimate: 2.749  (weeks-months)

 Advection Times (hr):
    Air:      100
    Water:    1000
    Sediment: 5e+004
```

A.8.2 Release to Water

Run Date: 2024-06-21

```
CAS Number: 000084-61-7
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)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(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
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(=O)O  [ester, aromatic attach]         |-0.7121  | -1.4242
 Const |     |  Equation Constant                         |         |  0.2290
-------+-----+--------------------------------------------+---------+--------
                                                  Log Kow   =   6.2026

MPBPVP (v1.43) Program Results:
===============================
Experimental Database Structure Match:
  Name     :  DICYCLOHEXYL PHTHALATE
```

```
  CAS Num  :  000084-61-7
  Exp MP (deg C):  66
  Exp BP (deg C):  224 @ 4 mm Hg
  Exp VP (mm Hg):  8.69E-07  (extrapolated)
         (Pa   ):  1.16E-004
  Exp VP (deg C):  25
  Exp VP ref    :  WERNER,AC (1952)

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)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)
      :  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)
  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 |  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
============+====================+==========+=========
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
-------------------------------------------------------

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group | 10  |  -CH2- (ring)      |    7.75  |   77.50
 Group |  2  |  >CH-  (ring)      |   19.88  |   39.76
 Group |  2  |  -COO- (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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
---------------------------------- WSKOW v1.43 Results -----------------------
Log Kow  (estimated)  :  6.20
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  4.82 (user entered)

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 deg C (Use Tm = 25 for all liquids)

      Correction(s):         Value
      --------------------   -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -5.349
   Water Solubility at 25 deg C (mg/L):  1.48


WATERNT Program (v1.01) Results:
===============================

                  Water Sol (v1.01 est): 2.4027 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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
-------+-----+--------------------------------------------+----------+---------
 TYPE  | NUM |    WATER SOLUBILITY FRAGMENT DESCRIPTION   |  COEFF   |  VALUE  
-------+-----+--------------------------------------------+----------+---------
 Frag  |  2  |  -CH     [aliphatic carbon]                |-0.5285   | -1.0570
 Frag  |  4  |  Aromatic Carbon  (C-H type)               |-0.3359   | -1.3435
 Frag  |  2  |  -C(=O)O  [ester, aromatic attach]         | 0.7006   |  1.4012
 Frag  |  2  |  Aromatic Carbon  (C-substituent type)     |-0.5400   | -1.0799
 Frag  | 10  |  -CH2-  [aliphatic carbon, cyclic]         |-0.3308   | -3.3084
 Const |     |  Equation Constant                         |          |  0.2492
-------+-----+--------------------------------------------+----------+---------
                              Log Water Sol (moles/L) at 25 dec C  =   -5.1384
                              Water Solubility (mg/L) at 25 dec C  =   2.4027


ECOSAR Program (v1.11) Results:
===============================
ECOSAR Version 1.11 Results Page

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

```
CAS Num:
ChemID1:
MOL FOR: C20 H26 O4
MOL WT : 330.43
Log Kow: 6.203      (EpiSuite Kowwin v1.68 Estimate)
Log Kow:            (User Entered)
Log Kow:            (PhysProp DB exp value - for comparison only)
Melt Pt: 66.00      (deg C, User Entered for Wat Sol estimate)
Melt Pt: 66.00      (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 0.06964    (mg/L, EpiSuite WSKowwin v1.43 Estimate)
Wat Sol: 1.48       (mg/L, User Entered)
Wat Sol: 4          (mg/L, PhysProp DB exp value)

 --------------------------------------
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
                                                                    Predicted
ECOSAR Class                 Organism            Duration  End Pt   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)                    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)


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

----------+---------------------------------------------+---------+----------
   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
----------+---------------------------------------------+---------+----------
 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)                       |            | -1.50
        |           2  CH (C)(C)(O)                     |            |  0.24
        |           4  Car-H (Car)(Car)                 |            |  0.44
        |           2  Car (Car)(Car)(CO)               |            | -1.68
        |           2  CO (O)(Car)                      |            |  9.14
        |           2  O (C)(CO)                        |            | -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:
======================================

          Log Koa: 10.233

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
--------------------------- KOAWIN v1.10 Results --------------------------

Log Koa (octanol/air) estimate:  10.233
    Koa (octanol/air) estimate:  1.711e+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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 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
   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(=O)-O-C]                      | 0.1742  |  0.3484
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.1573
 Const|  *  |  Equation Constant                         |         |  0.7475
============+============================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)     |         |  0.9386
============+============================================+=========+=========

------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION         |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-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
------+-----+--------------------------------------------+---------+---------
```

```
 Frag |  2  |  Ester   [-C(=O)-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(=O)-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        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  0.2319 |  0.4638
 Frag |  4  |  Aromatic-H                                |  0.0004 |  0.0016
 Frag | 10  |  -CH2-  [cyclic]                           |  0.0141 |  0.1411
 Frag |  2  |  -CH -  [cyclic]                           |  0.0079 |  0.0158
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.5211
 Const|  *  |  Equation Constant                         |         |  0.5544
============+============================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)  |         |  0.6556
============+============================================+=========+=========

------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin6 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  1.5833 |  3.1665
 Frag |  4  |  Aromatic-H                                |  0.0342 |  0.1368
 Frag | 10  |  -CH2-  [cyclic]                           |  0.1206 |  1.2058
 Frag |  2  |  -CH -  [cyclic]                           |  0.0294 |  0.0589
 MolWt|  *  |  Molecular Weight Parameter                |         | -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


------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin7 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  0.1719 |  0.3437
 Frag |  4  |  Aromatic-H                                | -0.0954 | -0.3817
 Frag | 10  |  -CH2-  [cyclic]                           | -0.1200 | -1.2001
 Frag |  2  |  -CH -  [cyclic]                           |  0.0395 |  0.0789
 Const|  *  |  Equation Constant                         |         |  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
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.


BioHCwin (v1.01) Program Results:
==============================
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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)):
       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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   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


KOCWIN Program (v2.00) Results:
==============================
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
```

```
MOL FOR: C20 H26 O4
MOL WT : 330.43
--------------------------- KOCWIN v2.01 Results ---------------------------

  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):
                  2   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   )  ......................... :  4.82
         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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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 "**".

ESTER:  R1-C(=O)-O-R2                ** R1: -Phenyl
                                        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(=O)-O-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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 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:
===========================================================
------+-----+--------------------------------------------+---------+---------
 TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      | -0.7605 | -1.5211
 Frag |  4  |  Aromatic-H                                |  0.2664 |  1.0655
 Frag | 10  |  -CH2-  [cyclic]                           |  0.0963 |  0.9625
 Frag |  2  |  -CH -  [cyclic]                           |  0.0126 |  0.0252
 Frag |  1  |  Benzene                                   | -0.4277 | -0.4277
 L Kow|  *  |  Log Kow =   4.82 (user-entered   )        |  0.3073 |  1.4814
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.8473
 Const|  *  |  Equation Constant                         |         | -1.5371
============+============================================+=========+=========
   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   |
============+============================================+=========+=========

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)

                             RIVER             LAKE
                           ---------         ---------
Water Depth     (meters):   1                 1
Wind Velocity    (m/sec):   5                 0.5
Current Velocity (m/sec):   1                 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
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
          -Aeration tank       0.00      9635.43       10000.00
          -Settling tank       0.00      9635.43       10000.00

 STP Overall Chemical Mass Balance:
 ---------------------------------
                            g/h               mol/h          percent

Influent                   1.00E+001         3.0E-002        100.00

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

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 (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
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       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+000         1.2E-002         38.51
Waste sludge                2.37E-001         7.2E-004          2.37
Primary volatilization      1.25E-005         3.8E-008          0.00
Settling volatilization     3.02E-006         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
Settling biodegradation     3.10E-001         9.4E-004          3.10
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+000         2.9E-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)
  Melting Pt  : 66 deg C (user-entered)
  Log Kow     : 4.82  (user-entered)
  Soil Koc    : 1.33e+004  (KOCWIN MCI method)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.000513        10.6         0
   Water     56.5            900          1000
   Soil      0.0338          1.8e+003     0
   Sediment  43.5            8.1e+003     0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       2.58e-015    0.321       0.049       0.0321      0.0049
   Water     7.54e-013    416         540         41.6        54
   Soil      1.6e-017     0.124       0           0.0124      0
   Sediment  9.25e-013    35.5        8.31        3.55        0.831

   Persistence Time: 956 hr
   Reaction Time:    2.12e+003 hr
   Advection Time:   1.74e+003 hr
   Percent Reacted:  45.2
   Percent Advected: 54.8

   Water Compartment Percents:
   --------------------------
           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.000513        10.6         0
   Water     56.5            900          1000
     water     (55.2)
     biota     (0.182)
     suspended sediment (1.1)
   Soil      0.0338          1.8e+003     0
   Sediment  43.5            8.1e+003     0

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      10.58
      Water:    900
      Soil:     1800
      Sediment: 8100
```

```
        Biowin estimate: 2.749  (weeks-months)
    Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004


Level III Fugacity Model (Full-Output): EQC Default
=====================================================
  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)
  Melting Pt  : 66 deg C (user-entered)
  Log Kow     : 4.82  (user-entered)
  Soil Koc    : 2.71e+004  (EQC Model Default)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air      0.00035         10.6         0
   Water    39.3            900          1000
   Soil     0.0231          1.8e+003     0
   Sediment 60.6            8.1e+003     0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air      2.42e-015    0.301       0.046       0.0301      0.0046
   Water    7.08e-013    398         517         39.8        51.7
   Soil     7.42e-018    0.117       0           0.0117      0
   Sediment 8.75e-013    68.2        15.9        6.82        1.59

   Persistence Time: 1.31e+003 hr
   Reaction Time:    2.82e+003 hr
   Advection Time:   2.47e+003 hr
   Percent Reacted:  46.7
   Percent Advected: 53.3

   Water Compartment Percents:
   --------------------------
           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air      0.00035         10.6         0
   Water    39.3            900          1000
     water     (37.7)
     biota     (0.124)
     suspended sediment (1.53)
   Soil     0.0231          1.8e+003     0
   Sediment 60.6            8.1e+003     0

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      10.58
      Water:    900
      Soil:     1800
      Sediment: 8100
        Biowin estimate: 2.749  (weeks-months)

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004
```

A.8.3 Release to Soil

Run Date: 2024-06-21

```
CAS Number: 000084-61-7
```

```
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)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(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
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(=O)O  [ester, aromatic attach]         |-0.7121  | -1.4242
 Const |     |  Equation Constant                         |         |  0.2290
-------+-----+--------------------------------------------+---------+--------
                                                           Log Kow   =   6.2026


MPBPVP (v1.43) Program Results:
===============================
Experimental Database Structure Match:
  Name     :  DICYCLOHEXYL PHTHALATE
  CAS Num  :  000084-61-7
  Exp MP (deg C):  66
  Exp BP (deg C):  224 @ 4 mm Hg
  Exp VP (mm Hg):  8.69E-07  (extrapolated)
         (Pa   ):  1.16E-004
  Exp VP (deg C):  25
  Exp VP ref    :  WERNER,AC (1952)

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)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)
      :  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)
  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 |  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
=============+====================+==========+=========
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
-------------------------------------------------------

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group | 10  |  -CH2- (ring)      |    7.75  |   77.50
 Group |  2  |  >CH-  (ring)      |   19.88  |   39.76
 Group |  2  |  -COO- (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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
---------------------------------- WSKOW v1.43 Results ------------------------
Log Kow  (estimated)  :  6.20
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  4.82 (user entered)

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 deg C (Use Tm = 25 for all liquids)

      Correction(s):         Value
      --------------------   -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -5.349
   Water Solubility at 25 deg C (mg/L):  1.48
```

```
WATERNT Program (v1.01) Results:
===============================

                  Water Sol (v1.01 est): 2.4027 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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
-------+-----+--------------------------------------------+----------+---------
 TYPE  | NUM |    WATER SOLUBILITY FRAGMENT DESCRIPTION    |  COEFF   |  VALUE
-------+-----+--------------------------------------------+----------+---------
 Frag  |  2  |  -CH     [aliphatic carbon]                |-0.5285   | -1.0570
 Frag  |  4  |  Aromatic Carbon  (C-H type)               |-0.3359   | -1.3435
 Frag  |  2  |  -C(=O)O  [ester, aromatic attach]         | 0.7006   |  1.4012
 Frag  |  2  |  Aromatic Carbon  (C-substituent type)     |-0.5400   | -1.0799
 Frag  | 10  |  -CH2-  [aliphatic carbon, cyclic]         |-0.3308   | -3.3084
 Const |     |  Equation Constant                         |          |  0.2492
-------+-----+--------------------------------------------+----------+---------
                              Log Water Sol (moles/L) at 25 dec C  =   -5.1384
                              Water Solubility (mg/L) at 25 dec C  =   2.4027


ECOSAR Program (v1.11) Results:
===============================
ECOSAR Version 1.11 Results Page

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
CAS Num:
ChemID1:
MOL FOR: C20 H26 O4
MOL WT : 330.43
Log Kow: 6.203      (EpiSuite Kowwin v1.68 Estimate)
Log Kow:            (User Entered)
Log Kow:            (PhysProp DB exp value - for comparison only)
Melt Pt: 66.00      (deg C, User Entered for Wat Sol estimate)
Melt Pt: 66.00      (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 0.06964    (mg/L, EpiSuite WSKowwin v1.43 Estimate)
Wat Sol: 1.48       (mg/L, User Entered)
Wat Sol: 4          (mg/L, PhysProp DB exp value)


--------------------------------------
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
                                                                   Predicted
ECOSAR Class                 Organism           Duration   End Pt   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)                   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)


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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 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
----------+---------------------------------------------+---------+----------
   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
```

```
----------+---------------------------------------------+---------+---------
 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)                     |            | -1.50
        |           2  CH (C)(C)(O)                   |            |  0.24
        |           4  Car-H (Car)(Car)               |            |  0.44
        |           2  Car (Car)(Car)(CO)             |            | -1.68
        |           2  CO (O)(Car)                    |            |  9.14
        |           2  O (C)(CO)                      |            | -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:
======================================

          Log Koa: 10.233

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
--------------------------- KOAWIN v1.10 Results -------------------------

Log Koa (octanol/air) estimate:  10.233
    Koa (octanol/air) estimate:  1.711e+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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 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
   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(=O)-O-C]                      | 0.1742  |  0.3484
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.1573
 Const|  *  |  Equation Constant                         |         |  0.7475
============+============================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)     |         |  0.9386
============+============================================+=========+=========

------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin2 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-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
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-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(=O)-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        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      | 0.2319  |  0.4638
 Frag |  4  |  Aromatic-H                                | 0.0004  |  0.0016
 Frag | 10  |  -CH2-  [cyclic]                           | 0.0141  |  0.1411
 Frag |  2  |  -CH -  [cyclic]                           | 0.0079  |  0.0158
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.5211
 Const|  *  |  Equation Constant                         |         |  0.5544
============+============================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)  |         |  0.6556
============+============================================+=========+=========

------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin6 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      | 1.5833  |  3.1665
```

```
 Frag |  4  |  Aromatic-H                                 |  0.0342 |  0.1368
 Frag | 10  |  -CH2-  [cyclic]                            |  0.1206 |  1.2058
 Frag |  2  |  -CH -  [cyclic]                            |  0.0294 |  0.0589
 MolWt|  *  |  Molecular Weight Parameter                 |         | -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


------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin7 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  0.1719 |  0.3437
 Frag |  4  |  Aromatic-H                                | -0.0954 | -0.3817
 Frag | 10  |  -CH2-  [cyclic]                           | -0.1200 | -1.2001
 Frag |  2  |  -CH -  [cyclic]                           |  0.0395 |  0.0789
 Const|  *  |  Equation Constant                         |         |  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
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.


BioHCwin (v1.01) Program Results:
============================
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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)):
       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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   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


KOCWIN Program (v2.00) Results:
==============================
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
--------------------------  KOCWIN v2.01 Results  --------------------------

  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):
                  2   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   )  ......................... :  4.82
         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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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 "**".

ESTER:  R1-C(=O)-O-R2                 ** R1: -Phenyl
                                         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(=O)-O-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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 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:
===========================================================
------+-----+--------------------------------------------+---------+---------
 TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      | -0.7605 | -1.5211
 Frag |  4  |  Aromatic-H                                |  0.2664 |  1.0655
 Frag | 10  |  -CH2-  [cyclic]                           |  0.0963 |  0.9625
 Frag |  2  |  -CH -  [cyclic]                           |  0.0126 |  0.0252
 Frag |  1  |  Benzene                                   | -0.4277 | -0.4277
 L Kow|  *  |  Log Kow =   4.82 (user-entered   )        |  0.3073 |  1.4814
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.8473
 Const|  *  |  Equation Constant                         |         | -1.5371
============+============================================+=========+=========
   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   |
============+============================================+=========+=========

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)

                             RIVER            LAKE
                           ---------        ---------
Water Depth     (meters):   1                1
Wind Velocity    (m/sec):   5                0.5
Current Velocity (m/sec):   1                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
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
          -Aeration tank       0.00      9635.43       10000.00
          -Settling tank       0.00      9635.43       10000.00

 STP Overall Chemical Mass Balance:
 ---------------------------------
                             g/h               mol/h          percent

Influent                    1.00E+001         3.0E-002       100.00

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

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 (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
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       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+000         1.2E-002        38.51
Waste sludge                2.37E-001         7.2E-004         2.37
Primary volatilization      1.25E-005         3.8E-008         0.00
Settling volatilization     3.02E-006         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
Settling biodegradation     3.10E-001         9.4E-004         3.10
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+000         2.9E-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)
  Melting Pt  : 66 deg C (user-entered)
  Log Kow     : 4.82  (user-entered)
  Soil Koc    : 1.33e+004  (KOCWIN MCI method)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air        9.98e-005      10.6          0
   Water      0.0477         900           0
```

```
   Soil      99.9           1.8e+003     1000
   Sediment  0.0367         8.1e+003     0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       1.36e-015    0.17        0.0259      0.017       0.00259
   Water     1.73e-015    0.952       1.24        0.0952      0.124
   Soil      1.29e-013    998         0           99.8        0
   Sediment  2.12e-015    0.0814      0.019       0.00814     0.0019

   Persistence Time: 2.59e+003 hr
   Reaction Time:    2.6e+003 hr
   Advection Time:   2.02e+006 hr
   Percent Reacted:  99.9
   Percent Advected: 0.128

   Water Compartment Percents:
   --------------------------
           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       9.98e-005      10.6          0
   Water     0.0477         900           0
     water     (0.0466)
     biota     (0.000154)
     suspended sediment (0.000931)
   Soil      99.9           1.8e+003     1000
   Sediment  0.0367         8.1e+003     0

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      10.58
      Water:    900
      Soil:     1800
      Sediment: 8100
        Biowin estimate: 2.749  (weeks-months)

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004


Level III Fugacity Model (Full-Output): EQC Default
=====================================================
  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)
  Melting Pt  : 66 deg C (user-entered)
  Log Kow     : 4.82  (user-entered)
  Soil Koc    : 2.71e+004  (EQC Model Default)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       4.91e-005      10.6          0
   Water     0.0251         900           0
   Soil      99.9           1.8e+003     1000
   Sediment  0.0387         8.1e+003     0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       6.7e-016     0.0836      0.0128      0.00836     0.00128
   Water     8.92e-016    0.502       0.652       0.0502      0.0652
   Soil      6.33e-014    999         0           99.9        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
```

```
   Advection Time:   3.79e+006 hr
   Percent Reacted:  99.9
   Percent Advected: 0.0685

   Water Compartment Percents:
   --------------------------
           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       4.91e-005       10.6          0
   Water     0.0251          900           0
     water     (0.0241)
     biota     (7.95e-005)
     suspended sediment (0.000977)
   Soil      99.9            1.8e+003     1000
   Sediment  0.0387          8.1e+003     0

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      10.58
      Water:    900
      Soil:     1800
      Sediment: 8100
        Biowin estimate: 2.749  (weeks-months)

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004
```

A.8.4 Release to Air, Water, and Soil

Run Date: 2024-06-21

```
CAS Number: 000084-61-7
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)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(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
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(=O)O  [ester, aromatic attach]         |-0.7121  | -1.4242
 Const |     |  Equation Constant                         |         |  0.2290
-------+-----+--------------------------------------------+---------+--------
                                                           Log Kow   =   6.2026
```

```
MPBPVP (v1.43) Program Results:
===============================
Experimental Database Structure Match:
  Name     :  DICYCLOHEXYL PHTHALATE
  CAS Num  :  000084-61-7
  Exp MP (deg C):  66
  Exp BP (deg C):  224 @ 4 mm Hg
  Exp VP (mm Hg):  8.69E-07  (extrapolated)
         (Pa   ):  1.16E-004
  Exp VP (deg C):  25
  Exp VP ref    :  WERNER,AC (1952)

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)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)
      :  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)
  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 |  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 
============+====================+==========+=========
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 
-------------------------------------------------------

-------+-----+--------------------+----------+---------
 TYPE  | NUM |  MELT DESCRIPTION  |  COEFF   |  VALUE  
-------+-----+--------------------+----------+---------
 Group | 10  |  -CH2- (ring)      |    7.75  |   77.50 
 Group |  2  |  >CH-  (ring)      |   19.88  |   39.76 
 Group |  2  |  -COO- (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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
---------------------------------- WSKOW v1.43 Results ------------------------
Log Kow  (estimated)  :  6.20
Log Kow (experimental):  not available from database
Log Kow used by Water solubility estimates:  4.82 (user entered)

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 deg C (Use Tm = 25 for all liquids)

      Correction(s):         Value
      --------------------   -----
       No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :  -5.349
   Water Solubility at 25 deg C (mg/L):  1.48


WATERNT Program (v1.01) Results:
===============================

                  Water Sol (v1.01 est): 2.4027 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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
-------+-----+---------------------------------------------+----------+---------
 TYPE  | NUM |    WATER SOLUBILITY FRAGMENT DESCRIPTION    |  COEFF   |  VALUE
-------+-----+---------------------------------------------+----------+---------
 Frag  |  2  | -CH     [aliphatic carbon]                  |-0.5285   | -1.0570
 Frag  |  4  | Aromatic Carbon  (C-H type)                 |-0.3359   | -1.3435
 Frag  |  2  | -C(=O)O  [ester, aromatic attach]           | 0.7006   |  1.4012
 Frag  |  2  | Aromatic Carbon  (C-substituent type)       |-0.5400   | -1.0799
 Frag  | 10  | -CH2-  [aliphatic carbon, cyclic]           |-0.3308   | -3.3084
 Const |     | Equation Constant                           |          |  0.2492
-------+-----+---------------------------------------------+----------+---------
                              Log Water Sol (moles/L) at 25 dec C  =   -5.1384
                              Water Solubility (mg/L) at 25 dec C  =   2.4027
```

```
ECOSAR Program (v1.11) Results:
===============================
ECOSAR Version 1.11 Results Page

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
CAS Num:
ChemID1:
MOL FOR: C20 H26 O4
MOL WT : 330.43
Log Kow: 6.203      (EpiSuite Kowwin v1.68 Estimate)
Log Kow:            (User Entered)
Log Kow:            (PhysProp DB exp value - for comparison only)
Melt Pt: 66.00      (deg C, User Entered for Wat Sol estimate)
Melt Pt: 66.00      (deg C, PhysProp DB exp value for Wat Sol est)
Wat Sol: 0.06964    (mg/L, EpiSuite WSKowwin v1.43 Estimate)
Wat Sol: 1.48       (mg/L, User Entered)
Wat Sol: 4          (mg/L, PhysProp DB exp value)


--------------------------------------
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
                                                                  Predicted
ECOSAR Class                 Organism            Duration  End Pt   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)                    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)


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

----------+---------------------------------------------+---------+----------
   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
----------+---------------------------------------------+---------+----------
 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)                       |            | -1.50
        |           2  CH (C)(C)(O)                     |            |  0.24
        |           4  Car-H (Car)(Car)                 |            |  0.44
        |           2  Car (Car)(Car)(CO)               |            | -1.68
        |           2  CO (O)(Car)                      |            |  9.14
        |           2  O (C)(CO)                        |            | -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:
======================================

          Log Koa: 10.233

SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
--------------------------- KOAWIN v1.10 Results ---------------------------

Log Koa (octanol/air) estimate:  10.233
    Koa (octanol/air) estimate:  1.711e+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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 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
   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(=O)-O-C]                       | 0.1742  |  0.3484
 MolWt|  *  |  Molecular Weight Parameter                 |         | -0.1573
 Const|  *  |  Equation Constant                          |         |  0.7475
============+============================================+=========+=========
   RESULT   |    Biowin1 (Linear Biodeg Probability)      |         |  0.9386
============+============================================+=========+=========

------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin2 FRAGMENT DESCRIPTION         |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-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
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-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(=O)-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        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  0.2319 |  0.4638
 Frag |  4  |  Aromatic-H                                |  0.0004 |  0.0016
 Frag | 10  |  -CH2-  [cyclic]                           |  0.0141 |  0.1411
 Frag |  2  |  -CH -  [cyclic]                           |  0.0079 |  0.0158
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.5211
 Const|  *  |  Equation Constant                         |         |  0.5544
============+============================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)  |         |  0.6556
============+============================================+=========+=========

------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin6 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  1.5833 |  3.1665
 Frag |  4  |  Aromatic-H                                |  0.0342 |  0.1368
 Frag | 10  |  -CH2-  [cyclic]                           |  0.1206 |  1.2058
 Frag |  2  |  -CH -  [cyclic]                           |  0.0294 |  0.0589
 MolWt|  *  |  Molecular Weight Parameter                |         | -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


------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |        Biowin7 FRAGMENT DESCRIPTION        |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  0.1719 |  0.3437
 Frag |  4  |  Aromatic-H                                | -0.0954 | -0.3817
 Frag | 10  |  -CH2-  [cyclic]                           | -0.1200 | -1.2001
 Frag |  2  |  -CH -  [cyclic]                           |  0.0395 |  0.0789
 Const|  *  |  Equation Constant                         |         |  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
 degradation in the OECD301C test only; using data from the Chemicals
 Evaluation and Research Institute Japan (CERIJ) database.


BioHCwin (v1.01) Program Results:
==============================
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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)):
       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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   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
```

```
KOCWIN Program (v2.00) Results:
==============================
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 1,2-Benzenedicarboxylic acid, dicyclohexyl ester
MOL FOR: C20 H26 O4
MOL WT : 330.43
---------------------------  KOCWIN v2.01 Results  ---------------------------

  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):
                  2   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   )  ......................... :  4.82
         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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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 "**".

ESTER:  R1-C(=O)-O-R2                ** R1: -Phenyl
                                        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(=O)-O-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 : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(CCCC3)C3)c2
CHEM   : 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:
===========================================================
------+-----+--------------------------------------------+---------+---------
 TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      | -0.7605 | -1.5211
 Frag |  4  |  Aromatic-H                                |  0.2664 |  1.0655
 Frag | 10  |  -CH2-  [cyclic]                           |  0.0963 |  0.9625
 Frag |  2  |  -CH -  [cyclic]                           |  0.0126 |  0.0252
 Frag |  1  |  Benzene                                   | -0.4277 | -0.4277
 L Kow|  *  |  Log Kow =   4.82 (user-entered   )        |  0.3073 |  1.4814
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.8473
 Const|  *  |  Equation Constant                         |         | -1.5371
============+============================================+=========+=========
   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   |
============+============================================+=========+=========

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)
                             RIVER             LAKE
                           ---------         ---------
Water Depth     (meters):   1                 1
Wind Velocity    (m/sec):   5                 0.5
Current Velocity (m/sec):   1                 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
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
          -Aeration tank       0.00      9635.43       10000.00
          -Settling tank       0.00      9635.43       10000.00

 STP Overall Chemical Mass Balance:
 ---------------------------------
                             g/h               mol/h          percent

Influent                    1.00E+001         3.0E-002        100.00

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

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 (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
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       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+000         1.2E-002       38.51
Waste sludge                 2.37E-001         7.2E-004        2.37
Primary volatilization       1.25E-005         3.8E-008        0.00
Settling volatilization      3.02E-006         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
Settling biodegradation      3.10E-001         9.4E-004        3.10
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+000         2.9E-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)
  Melting Pt  : 66 deg C (user-entered)
  Log Kow     : 4.82  (user-entered)
  Soil Koc    : 1.33e+004  (KOCWIN MCI method)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.228           10.6          1000
   Water     13.2            900           1000
   Soil      76.4            1.8e+003      1000
   Sediment  10.2            8.1e+003      0

             Fugacity    Reaction     Advection    Reaction     Advection
              (atm)      (kg/hr)       (kg/hr)     (percent)    (percent)
   Air       5.06e-012    630          96.2         21           3.21
   Water     7.79e-013    429          557          14.3         18.6
   Soil      1.6e-013     1.24e+003    0            41.4         0
   Sediment  9.55e-013    36.7         8.57         1.22         0.286

   Persistence Time: 1.41e+003 hr
   Reaction Time:    1.81e+003 hr
   Advection Time:   6.37e+003 hr
   Percent Reacted:  77.9
   Percent Advected: 22.1

   Water Compartment Percents:
   --------------------------
           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.228           10.6          1000
   Water     13.2            900           1000
     water     (12.9)
     biota     (0.0426)
     suspended sediment (0.258)
   Soil      76.4            1.8e+003      1000
   Sediment  10.2            8.1e+003      0
```

```
   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      10.58
      Water:    900
      Soil:     1800
      Sediment: 8100
        Biowin estimate: 2.749  (weeks-months)

   Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004


Level III Fugacity Model (Full-Output): EQC Default
=====================================================
  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)
  Melting Pt  : 66 deg C (user-entered)
  Log Kow     : 4.82  (user-entered)
  Soil Koc    : 2.71e+004  (EQC Model Default)

           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.209         10.6          1000
   Water     11.6          900           1000
   Soil      70.3          1.8e+003      1000
   Sediment  17.9          8.1e+003      0

             Fugacity    Reaction    Advection   Reaction    Advection
              (atm)      (kg/hr)      (kg/hr)    (percent)   (percent)
   Air       5.05e-012    630         96.2        21          3.21
   Water     7.3e-013     411         533         13.7        17.8
   Soil      7.88e-014    1.24e+003   0           41.4        0
   Sediment  9.02e-013    70.3        16.4        2.34        0.548

   Persistence Time: 1.53e+003 hr
   Reaction Time:    1.95e+003 hr
   Advection Time:   7.11e+003 hr
   Percent Reacted:  78.5
   Percent Advected: 21.5

   Water Compartment Percents:
   --------------------------
           Mass Amount    Half-Life    Emissions
            (percent)        (hr)       (kg/hr)
   Air       0.209         10.6          1000
   Water     11.6          900           1000
     water     (11.1)
     biota     (0.0367)
     suspended sediment (0.452)
   Soil      70.3          1.8e+003      1000
   Sediment  17.9          8.1e+003      0

   Half-Lives (hr), (based upon Biowin (Ultimate) and Aopwin):
      Air:      10.58
      Water:    900
      Soil:     1800
      Sediment: 8100
        Biowin estimate: 2.749  (weeks-months)
    Advection Times (hr):
      Air:      100
      Water:    1000
      Sediment: 5e+004
```

A.9 Atmospheric Oxidation Rate (AOPWIN)

Run Date: 2024-06-21

```
SMILES : O=C(OC(CCCC1)C1)c(c(ccc2)C(=O)OC(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
Addition to Fused Rings    =   0.0000 E-12 cm3/molecule-sec

   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

------------------------------------------------------------------------------
```

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

Run Date: 2024-06-21

```
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
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
          -Aeration tank      0.00      9635.43       10000.00
          -Settling tank      0.00      9635.43       10000.00

 STP Overall Chemical Mass Balance:
 ---------------------------------
                             g/h               mol/h          percent

Influent                    1.00E+001         3.0E-002        100.00

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

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 (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
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       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+000         1.2E-002        38.51
Waste sludge                2.37E-001         7.2E-004         2.37
Primary volatilization      1.25E-005         3.8E-008         0.00
Settling volatilization     3.02E-006         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
Settling biodegradation     3.10E-001         9.4E-004         3.10
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+000         2.9E-002        97.47
Total biodegradation        5.66E+000         1.7E-002        56.59
 (** Total removal recommended maximum is 95 percent)
```

A.11 Bioaccumulation Potential (BCFBAF)

Run Date: 2024-07-02

```
SMILES : C1CCC(CC1)OC(=O)c2ccccc2C(=O)OC3CCCCC3
CHEM   : Dicyclohexyl Phthalate
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)

=============================
```

```
BCF (Bioconcentration Factor):
=============================
Log Kow  (estimated)  :  6.20
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(=O)-O-C]                      | -0.7605 | -1.5211
 Frag |  4  |  Aromatic-H                                |  0.2664 |  1.0655
 Frag | 10  |  -CH2-  [cyclic]                           |  0.0963 |  0.9625
 Frag |  2  |  -CH -  [cyclic]                           |  0.0126 |  0.0252
 Frag |  1  |  Benzene                                   | -0.4277 | -0.4277
 L Kow|  *  |  Log Kow =   4.82 (user-entered   )        |  0.3073 |  1.4814
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.8473
 Const|  *  |  Equation Constant                         |         | -1.5371
============+============================================+=========+=========
   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   |
============+============================================+=========+=========

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)
```

A.12 Biodegradation Potential (BIOWIN)

Run Date: 2024-06-12.

```
SMILES : C1CCC(CC1)OC(=O)c2ccccc2C(=O)OC3CCCCC3
CHEM   : Dicyclohexyl Phthalate
MOL FOR: C20 H26 O4
MOL WT : 330.43
--------------------------- 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

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

------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |       Biowin2 FRAGMENT DESCRIPTION         |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-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
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-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(=O)-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         |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  0.2319 |  0.4638
 Frag |  4  |  Aromatic-H                                |  0.0004 |  0.0016
 Frag | 10  |  -CH2-  [cyclic]                           |  0.0141 |  0.1411
 Frag |  2  |  -CH -  [cyclic]                           |  0.0079 |  0.0158
 MolWt|  *  |  Molecular Weight Parameter                |         | -0.5211
 Const|  *  |  Equation Constant                         |         |  0.5544
============+============================================+=========+=========
   RESULT   |  Biowin5 (MITI Linear Biodeg Probability)  |         |  0.6556
============+============================================+=========+=========

------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |       Biowin6 FRAGMENT DESCRIPTION         |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  1.5833 |  3.1665
 Frag |  4  |  Aromatic-H                                |  0.0342 |  0.1368
 Frag | 10  |  -CH2-  [cyclic]                           |  0.1206 |  1.2058
```

```
 Frag |  2  |  -CH -  [cyclic]                            |  0.0294 |  0.0589
 MolWt|  *  |  Molecular Weight Parameter                 |         | -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


------+-----+--------------------------------------------+---------+---------
 TYPE | NUM |       Biowin7 FRAGMENT DESCRIPTION         |  COEFF  |  VALUE
------+-----+--------------------------------------------+---------+---------
 Frag |  2  |  Ester   [-C(=O)-O-C]                      |  0.1719 |  0.3437
 Frag |  4  |  Aromatic-H                                | -0.0954 | -0.3817
 Frag | 10  |  -CH2-  [cyclic]                           | -0.1200 | -1.2001
 Frag |  2  |  -CH -  [cyclic]                           |  0.0395 |  0.0789
 Const|  *  |  Equation Constant                         |         |  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
 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 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/m^3 (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/m^3 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. to 398 ng/m^3) (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/m^3 and the median concentration of 4.54 ng/m^3. 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/m^3 (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/m^3. Elevated concentrations in downtown regions were observed with a mean concentration of 95 ± 13 ng/m^3 (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/m^3 indoor, 95 ± 13 ng/m^3 outdoor) and non-congested (9 ± 3 ng/m^3 indoor, 110 ± 93 ng/m^3 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/m^3 (n.d. to 1923 ng/m^3) in newly constructed homes, 512 ng/m^3 (<37.2–787 ng/m^3) in existing homes, and 377 ng/m^3 (<7.2–1,257 ng/m^3) in office. DCHP was also detected in the dust and air particulate with a mean concentration of 627 ng/m^3 (<29.67–1,208 ng/m^3) in newly constructed homes, 667 ng/m^3 (<29.67–995 ng/m^3) in existing homes, and 502 ng/m^3 (71–1,197 ng/m^3) 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, Spain, identified DCHP in of samples with a mean outdoor atmospheric concentration of 9 ± 3 ng/m^3 (background) with elevated concentrations in downtown regions with a mean concentration of 12 ± 3 ng/m^3 (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 et al., 2020). Concentrations of DCHP were an order of magnitude lower than indoor DCHP concentration in both congested (95 ± 13 ng/m^3) and non-congested (110 ± 93 ng/m^3) 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/m^3 (<1–3.66 pg/m^3, n = 7) and 0.771 pg/m^3 (<1–1.17 pg/m^3, n = 8) in lakeside and urban regions, respectively (He et al., 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 (Başaran et al., 2020). Concentrations of all phthalates were highest in urban developed regions followed by industrial sites, near-road sites, and lowest concentrations in rural sites (Başaran et al., 2020).
- 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/m^3 (<0.02–0.03 ng/m^3), 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/m^3 (n.d. to 459 ng/m^3) in air and 130 ng/m^3 (n.d. to 485 ng/m^3) on dust (Ouyang et al., 2019).

B.3 Surface Water

Seven international studies have reported DCHP in surface water and suspended particulates. 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/m^3 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 Guangzhou, China identified 7 percent (n = 15) of urban lake samples with concentrations ranging from less than the method detection limit (MDL) to 0.076 µg/L and in 53 percent of benthic sediments with concentrations ranging from less than the MDL to 0.22 µg/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 proximity 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).
- Another 2005 survey of various surface water, municipal wastewater, and industrial wastewater

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 22 percent of effluent samples with concentration ranging from 2 to 20 ng/L. DCHP 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 33 percent of surface water samples with concentrations ranging from less than 3 to 60 ng/L, 47 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 from less than 2 to 11 ng/g dw (Vethaak et al., 2005).

B.4 Sediment

Three international studies identified DCHP in suspended sediments originating from China, The Netherlands, and Germany. The measured concentration ranges of DCHP measured in suspended sediment are listed below:

- 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).

Several studies reported DCHP measured in benthic sediments originating from China, Iran, South Korea, Kuwait, and The Netherlands; DCHP concentration ranges reported for each region are listed below:

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

B.5 Soil

Five chinese studies identified DCHP in soil, with concentrations ranged from 0.0058 to 11.8 µg/g dw of DCHP in soil (Zhang et al., 2019b; Niu et al., 2014; Liu et al., 2010; Zeng et al., 2009; Zeng et al., 2008b).

B.6 Biosolids

Three international studies have been identified pertaining to DCHP concentrations in wastewater biosolids:

- A survey of wastewater removal of phthalates in China identified DCHP in 100 percent of samples collected with concentrations ranging from 7.98 to 14.41 µg/L, with DCHP comprising between 6 to 19 percent of overall phthalate concentrations (Wu et al., 2019). Removal 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 accounting to 10 to 20 percent of the initial DCHP mass lost to biosolids sorption during wastewater treatment (Wu et al., 2019). Destruction of DCHP accounted for 51 to 56 percent of initial DCHP mass lost to destruction (Wu et al., 2019).

- 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) comprising 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 km^2 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; That study surveyed three wastewater treatment plants in china including removal from primary treatment, biological treatment (sequencing batch reactor [SBR], anaerobic-anoxic-oxic baffled bioreactor [AAOBR], and modified sequencing batch reactor [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 µg/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 ± 200 µg/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 µg/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 systems. Tertiary treatment, including filtration, chemical disinfection, and ultraviolet (UV) light disinfection, were not evaluated in this study.

An earlier (2005) survey of various surface water, municipal wastewater, and industrial wastewater 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 22 percent of effluent samples with concentrations ranging from 2 to 20 ng/L. DCHP was identified in 80 percent of untreated industrial wastewater with concentrations ranging from less than 5 to 19,000 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 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 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 g/kg (Lee et al., 2019).