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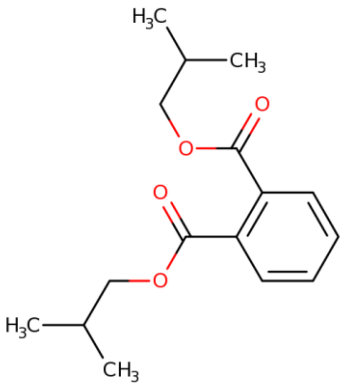
Pollution Prevention

# Draft Physical Chemistry and Fate and Transport Assessment for Di-isobutyl Phthalate (DIBP)

## Technical Support Document for the Draft Risk Evaluation

## CASRN: 84-69-5




***December 2024***

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# ABBREVIATIONS AND ACRONYMS

| | |
|---|---|
| ATSDR | Agency for Toxic Substances and Disease Registry |
| Atm | Atmospheres |
| atm·m$^3$/mol | Atmospheres – cubic meters per mole |
| BAF | Bioaccumulation factor |
| BCF | Bioconcentration factor |
| BMF | Biomagnification factor |
| BSAF | Biota-sediment accumulation factor |
| C | Celsius |
| CASRN | Chemical Abstract Service Registry Number |
| cP | Centipoise |
| DIBP | Di-isobutyl phthalate |
| dw | Dry weight |
| ECHA | European Chemicals Agency |
| EC/HC | Environment Canada and Health Canada |
| EPA | Environmental Protection Agency |
| F | Fahrenheit (°F) |
| g/cm$^3$ | Grams per cubic centimeter |
| HLC | Henry's Law constant |
| K | Kelvin |
| $K_{AW}$ | Air-water partition coefficient |
| $K_{OA}$ | Octanol-air partition coefficient |
| Koc | Organic carbon-water partition coefficient |
| $K_{OW}$ | Octanol-water partition coefficient |
| M | Molarity (mol/L = moles per Liter) |
| mg/L | Milligrams per liter |
| mL/min | Milliliters per minute |
| mmHg | Millimeters of mercury |
| mol | Mole |
| N/A | Not applicable |
| NCBI | National Center for Biotechnology Information |
| NIOSH | National Institute for Occupational Safety and Health |
| NLM | National Library of Medicine |
| nm | Nanometers |
| NR | Not reported |
| ·OH | Hydroxyl radical |
| Pa (hPa) | Pascals (hectopascals; 1 hPa = 100 Pa) |
| PA | Phthalic acid |
| pg/L | Picograms per liter |
| ppm | parts per million |
| QSAR | Quantitative structure activity relationship |
| RSC | Royal Society of Chemistry |
| RSD | Relative standard deviation |
| TSCA | Toxic Substances Control Act |
| TMF | Trophic magnification factor |
| U.S. | United States |
| UV (UV-Vis) | Ultraviolet (visible) light |
| ww | Wet weight |
| WWTP | Wastewater Treatment Plant |

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**Docket**

Supporting information can be found in the public docket, Docket ID EPA-HQ-OPPT-2018-0434.

**Disclaimer**

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**This draft technical support document was reviewed and cleared for release by OPPT and OCSPP leadership.**

# SUMMARY

This technical support document is in support of the *TSCA Draft Risk Evaluation for Di-isobutyl Phthalate (DIBP)*. EPA gathered and evaluated physical and chemical property data and information according to the process described in the *Draft Risk Evaluation for Di-isobutyl Phthalate (DIBP) – Systematic Review Protocol* (U.S. EPA, 2024c). During the evaluation of DIBP, 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 file *Draft Risk Evaluation for Di-isobutyl Phthalate (DIBP) – Systematic Review Supplemental File: Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties* (U.S. EPA, 2024b).

DIBP is a clear, viscous, and mostly odorless liquid (U.S. CPSC, 2011). As a branched phthalate ester, DIBP is used as plasticizer that melts around −64 °C (NLM, 2013). DIBP has a water solubility of 6.2 mg/L at 24°C (U.S. EPA, 2019) and a log $K_{OW}$ of 4.34 (Ishak et al., 2016). With a vapor pressure of $4.76\times10^{-5}$ mmHg at 25 °C and a boiling point of 296.5 °C (NLM, 2013), DIBP has the potential to be volatile from dry non-adsorbing surfaces. The selected Henry's Law Constant for DIBP is $1.83\times10^{-7}$ atm·$m^3$/mol at 25 °C (Elsevier, 2019).

In this document, EPA evaluated the reasonably available information to characterize the environmental fate and transport of DIBP. The key points are summarized below. Given the consistent results from numerous high-quality studies, there is robust evidence that DIBP:

- Is expected to undergo significant direct photolysis and will rapidly degrade in the atmosphere, with an indirect photochemical half-life of 27.6 hours (Section 4.3).
- Is not expected to appreciably hydrolyze under environmental conditions (Section 4.2).
- Is expected to have an environmental biodegradation half-life in aerobic environments on the order of days to weeks (Section 4.1).
- Is not expected to be subject to long range transport.
- Is expected to transform in the environment via biotic and abiotic processes to form phthalate monoesters, then phthalic acid, and ultimately biodegrade to form $CO_2$ and/or $CH_4$ (Section 4).
- Is expected to show strong affinity and sorption potential for organic carbon in soil and sediment (Section 3.2).
- Will be removed at rates between 65 and 95 percent in conventional wastewater treatment systems (Section 6.2).
- When released to air, will show strong affinity for adsorption to particulate matter, will mostly partition to soil and water, and remaining DIBP fraction will rapidly degrade in the atmosphere (Section 5.1).
- Is likely to be found in, and accumulate in, indoor dust (Section 5.1.1).

As a result of limited studies identified, there is moderate evidence that DIBP:

- Is unlikely to biodegrade under anoxic conditions and may persist in anaerobic soils and sediments (Section 4.1).
- Is not bioaccumulative in fish in the water column (Section 7).
- May be bioaccumulative in benthic organisms exposed to sediment with elevated concentrations of DIBP proximal to continual sources of release (Section 7).
- Is expected to be partially removed in conventional drinking water treatment systems via sorption to suspended organic matter and filtering media (Section 6.3).

# 1 INTRODUCTION

Diisobutyl phthalate (DIBP) is produced by the esterification of phthalic anhydride with isobutyl alcohol in the presence of an acid catalyst. DIBP is a member of the phthalate class of chemicals that are widely used as adhesives and sealants in the construction and automotive sector. DIBP is also commonly used in electronics, children's toys, and plastic and rubber materials. DIBP is considered ubiquitous in various environmental media due to its presence in both point and non-point source discharges from industrial and conventional wastewater treatment effluents, biosolids, and sewage sludge, stormwater runoff, and landfill leachate (Net et al., 2015).

This Physical Chemistry and Fate and Transport assessment was used to determine which environmental pathways to consider for DIBP's risk evaluation. Details on the environmental partitioning and media assessments can be found in Section 5. Briefly, based on DIBP's fate parameters, EPA anticipates DIBP to predominantly be found in water, soil, and sediment. DIBP in water is mostly attributable to discharges from industrial and municipal wastewater treatment plant effluent, surface water runoff, and, to a lesser degree, atmospheric deposition. Once in water, DIBP is expected to mostly partition to suspended organic matter and aquatic sediments. DIBP in soils is attributable to deposition from air and land application of biosolids.

EPA quantitatively assessed concentrations of DIBP in surface water, sediment, and soil from air to soil deposition. Ambient air concentrations were quantified for the purpose of estimating soil concentrations from air deposition but were not used for the exposure assessment as DIBP was not assumed to be persistent in the air ($t_{1/2}$ = 27.6 hours (U.S. EPA, 2017)). In addition, partitioning analysis showed DIBP partitions primarily to soil, compared to air, water, and sediment, even for air releases. Soil concentrations of DIBP from land applications were not quantitatively assessed in the screening level analysis as DIBP was expected to have limited persistence potential and mobility in soils receiving biosolids.

# 2 APPROACH AND METHODOLOGY FOR PHYSICAL AND CHEMICAL PROPERTY ASSESSMENT

EPA did a systematic review by conducting a literature search to find published physical and chemical property values available through 2019. Physical and chemical property data are extracted and evaluated for use in the risk evaluation as described in the Draft Systematic Review Protocol for DIBP (U.S. EPA, 2024c). Due to the large quantity of available data, only studies with an overall data quality ranking of High were selected for use in determining the representative physical and chemical properties of DIBP for the purposes of the risk evaluation. Experimentally derived values for a log $K_{OA}$ were not available and EPI Suite™ was used to estimate a value (U.S. EPA, 2017).

## 2.1 Selected Physical and Chemical Property Values for DIBP

**Table 2-1. Selected Physical and Chemical Property Values for DIBP**

| Property | Selected Value(s) | Reference(s) | Data Quality Rating |
|---|---|---|---|
| Molecular formula | $C_{16}H_{22}O_4$ | | |
| Molecular weight | 278.35 g/mol | | |
| Physical form | Clear Viscous Liquid | U.S. CPSC (2011) | High |
| Melting point | −64 °C | NLM (2013) | High |
| Boiling point | 296.5 °C | NLM (2013) | High |
| Density | 1.049 g/cm$^3$ | Rumble (2018) | High |
| Vapor pressure | 4.76E−05 mmHg | NLM (2013) | High |
| Vapor density | 9.59 | NCBI (2020) | High |
| Water solubility | 6.2 mg/L | U.S. EPA (2019) | High |
| Octanol/water partition coefficient (log $K_{OW}$) | 4.34 | Ishak et al. (2016) | High |
| Octanol/air partition coefficient (log $K_{OA}$) | 9.47 (EPI Suite™) | U.S. EPA (2017) | High |
| Henry's Law Constant | 1.83E−07 atm·m$^3$/mol at 25 °C | Elsevier (2019) | High |
| Flash point | 185 °C | Rumble (2018) | High |
| Autoflammability | 432 °C | NLM (2013) | High |
| Viscosity | 41 cP at 20 °C | NLM (2013) | High |

## 2.2 Endpoint Assessments

### 2.2.1 Melting Point

Melting point informs the chemical's physical state, environmental fate and transport, as well as the chemical's potential bioavailability. The EPA extracted and evaluated nine sources containing DIBP melting point information. Four of the sources were identified and evaluated as overall high-quality data sources. These sources reported DIBP melting points ranging from -82 to -37 °C (Elsevier, 2019; NLM, 2013; ECHA, 2012; Wang and Richert, 2007). The average of the reported melting point values within these sources is -60°C. EPA selected a melting point value of -64 °C (NLM, 2013) as a representative

melting point value closest to the average of the identified information from the overall high-quality data sources. The identified value is consistent with the value proposed in the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020).

### 2.2.2 Boiling Point

Boiling point informs the chemical's physical state, environmental fate and transport, as well as the chemical's potential bioavailability. The EPA extracted and evaluated ten data sources containing DIBP boiling point information. Six of the sources were identified and evaluated as overall high-quality data sources. These sources reported DIBP boiling points ranging from 296 to 327 °C (Elsevier, 2019; U.S. EPA, 2019; Rumble, 2018; NLM, 2013; ECHA, 2012; Wang and Richert, 2007). The mean of the reported boiling point values within these sources is 297.6 °C. EPA selected a boiling point value 296.5 °C (NLM, 2013) as the value that best represents the mean within the available high-quality sources under normal environmental conditions. The identified value is consistent with the value proposed in the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020).

### 2.2.3 Density

The EPA extracted and evaluated six data sources containing DIBP density information. Two of the sources were identified and evaluated as overall high-quality data sources. The overall high-quality sources reported DIBP density values of 1.036 to 1.049 g/cm$^3$ (Elsevier, 2019; Rumble, 2018). The mean of the reported density values is 1.044. EPA selected a density of 1.049 g/cm$^3$ (Rumble, 2018) to closely represent the mean of the density values obtained from the available data sources. The identified value is consistent with the value range proposed in the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020).

### 2.2.4 Vapor Pressure

Vapor pressure indicates the chemical's potential to volatilize, fugitive emissions and other releases to the atmosphere, undergo long range transport, and undergo specific exposure pathways. The EPA extracted and evaluated seven data sources containing DIBP vapor pressure information. Four of the sources were identified and evaluated as overall high-quality data sources. These sources reported DIBP vapor pressure ranging from $2.00\times10^{-6}$ to $5.80\times10^{-4}$ mmHg at 20 to 25 °C (Ishak et al., 2016; NLM, 2013; ECHA, 2012; Lu, 2009). The mean vapor pressure of the reported experimental vales at 25°C is $6.13\times10^{-4}$ mmHg. EPA selected the experimentally derived vapor pressure value of $4.76\times10^{-5}$ mmHg (NLM, 2013) to best represent the mean vapor pressure of DIBP obtained from the overall high-quality data sources under normal environmental conditions. The identified value is consistent with the value proposed in the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020).

### 2.2.5 Vapor Density

A data source providing vapor density of DIBP was not identified in the initial data review for the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020). The EPA has since identified one data source reporting DIBP vapor density. EPA extracted and evaluated the one data source, categorized as overall high-quality, which reported DIBP vapor density between 9.59 and 9.60 (NCBI, 2020). EPA is using the vapor density value of 9.59 from the one available data source as a representative value for normal environmental conditions.

### 2.2.6 Water Solubility

Water solubility informs many endpoints not only within the realm of fate and transport of DIBP in the environment, but also when modelling for industrial process, engineering, human and ecological hazard, and exposure assessments. The EPA extracted and evaluated twelve data sources containing DIBP water solubility information. Seven of the sources were identified and evaluated as overall high-quality data

sources. These sources reported water solubility values from 5.10 to 20.3 mg/L (U.S. EPA, 2019; EC/HC, 2017; NLM, 2013; ECHA, 2012; BASF, 2001; Hollifield, 1979). These data sources employed different experimental temperatures and analytical methods that might resulted in the wide range of water solubilities. Despite the wide range of water solubilities reported overall, the reported water solubility of DIBP at ambient temperature (24 to 25°C) is 5.1 to 9.6 mg/L. The mean of the reported water solubilities at near ambient temperature is 6.7 mg/L. A water solubility of 6.2 mg/L (U.S. EPA, 2019) was selected as the empirical value obtained from the overall high-quality data sources that best represents DIBP's mean water solubility under normal environmental conditions. The identified value is consistent with the value proposed in the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020).

### 2.2.7 Octanol/Water Partition Coefficient (log $K_{OW}$)

The octanol-water partition coefficient ($K_{OW}$) provides information on how the chemical will partition between octanol (which represents the lipids or fats in biota) and water. Kow informs on how the chemical is likely to partition in biological organisms as well as for the estimation of other properties including water solubility, bioconcentration, soil adsorption, and aquatic toxicity. The EPA extracted and evaluated seven data sources containing DIBP $K_{OW}$ information. Five of the sources were identified and evaluated as overall high-quality data sources. These sources reported DIBP log $K_{OW}$ ranging from 4.11 to 4.86 (Elsevier, 2019; U.S. EPA, 2019; Ishak et al., 2016; NLM, 2013; ECHA, 2012). The mean of the reported log $K_{OW}$ values is 4.31. EPA selected an experimental log $K_{OW}$ value of 4.34 (Ishak et al., 2016) as an approximate representation of the mean value obtained from the overall high-quality data sources under normal environmental conditions. The identified value is consistent with the value proposed in the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020).

### 2.2.8 Henry's Law Constant

The Henry's Law Constant (HLC) 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. The EPA extracted and evaluated four data sources containing DIBP Henry's Law Constant (HLC) information. Two of the sources were identified and evaluated as overall high-quality data sources. One overall high-quality data source reported an experimentally derived DIBP HLC value of $1.83\times10^{-7}$ (Elsevier, 2019). The second overall high-quality data source reported a HLC value of $1.31\times10^{-6}$ atm·m$^3$/mol (Cousins and Mackay, 2000), which was estimated with a quantitative structure–activity relationship model. EPA selected the experimental HLC value of $1.83\times10^{-7}$ atm·m$^3$/mol (Elsevier, 2019) for this risk evaluation. The identified value is consistent with the value proposed in the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020).

### 2.2.9 Flash Point

The EPA extracted and evaluated five data sources containing DIBP flash point information. Two of the sources were identified and evaluated as overall high-quality data sources. Both overall high-quality sources reported a DIBP flash point of 185 °C (Rumble, 2018; NLM, 2013). EPA selected a flash point value of 185 °C (Rumble, 2018) as the representative value of the available information identified from the overall high-quality data sources under normal environmental conditions. The selected value replaces the proposed flash point value in the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020). The data source used to obtain the flash point value of 169 °C proposed in the *Final Scope for the Risk Evaluation of DIBP* has been updated, and is now reporting a flash point value of 185 °C, consistent with the selected value for use in this risk evaluation.

### 2.2.10 Autoflammability

A value for the autoflammability of DIBP was not identified in the initial data review for the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020). The systematic review process conducted since identified one overall high-quality data source reporting an autoflammability value of 432 °C (NLM, 2013). The EPA selected an autoflammability value of 432 °C for DIBP (NLM, 2013) as the representative value.

### 2.2.11 Viscosity

The EPA extracted and evaluated one data source containing DIBP viscosity information. This source was identified and evaluated as an overall high-quality data source. This data source reported a viscosity value of 41 cP at 20 °C for DIBP (NLM, 2013). The EPA selected a value of 41 cP at 20 °C for DIBP's viscosity for this risk evaluation. The identified value is consistent with the value proposed in the *Final Scope for the Risk Evaluation of DIBP* (U.S. EPA, 2020).

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

The representative Physical and Chemical property values were selected based on professional judgement and the overall data quality ranking of the associated references. These physical and chemical property values are then used to inform chemical specific decisions across other disciplines. High quality data is preferred in the selection of physical and chemical properties. When few, or no high-quality studies are identified, a mix of high-medium studies, or medium studies may be used to inform selection. In some instances where no data were available, or there was a wide range of data that generally, but did not consistently agree with one another, models such as EPI Suite™ were used to estimate the value for the endpoint (*i.e.*, octanol-air partitioning coefficient) and cross checked with reported data from systematic review. The number and overall quality of the available data sources results in different confidence strength levels for the corresponding selected physical and chemical property values (U.S. EPA, 2021).

# 3 APPROACH AND METHODOLOGY FOR FATE AND TRANSPORT ASSESSMENT

In assessing the environmental fate and transport of DIBP, EPA considered reasonably available environmental fate data including biotic and abiotic biodegradation rates, removal during wastewater treatment, volatilization from lakes and rivers, and organic carbon:water partition coefficient (log $K_{OC}$). The full range of results from data sources that were rated high- and medium-quality were evaluated. Medium-quality data sources were considered for fate endpoints when no high-quality data sources were available.

Information on the full extracted data set is available in the file *Draft Risk Evaluation for Di-isobutyl Phthalate (DIBP) – Systematic Review Supplemental File: Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport* (U.S. EPA, 2024a). When no measured data were available from high- or medium-quality data sources, fate values were obtained from EPI Suite™ (U.S. EPA, 2017), a predictive tool for physical and chemical properties and environmental fate estimation. Information regarding the model inputs is available in Section 3.2.1.

Table 3-1 provides a summary of the selected data that EPA considered while assessing the environmental fate of DIBP and were updated after publication of *Final Scope of the Risk Evaluation for Di-isobutyl Phthalate (DIBP) CASRN 84-69-5* (U.S. EPA, 2020) with additional information identified through the systematic review process.

**Table 3-1. Summary of Environmental Fate Values for DIBP**

| Parameter | Selected Value(s) | Reference(s) |
|---|---|---|
| Octanol:Water Partition Coefficient (Log $K_{OW}$) | 4.34 | Ishak et al. (2016) |
| Organic Carbon:Water Partition Coefficient (Log $K_{OC}$) | 2.67 (average of 2.50, 2.56, and 2.86) | He et al. (2019) |
| Adsorption Coefficient (Log $K_d$) | 2.65-3.10 (suspended particulate matter/water) | Li et al. (2017a) |
| | 3.97-4.30 (sediment/water) | |
| Octanol:Air Partition Coefficient (Log $K_{OA}$) | 9.47 (EPI Suite estimate) | U.S. EPA (2017) |
| Air:Water Partition Coefficient (Log $K_{AW}$) | -4.3 (estimated) | Lu (2009) |
| | -4.27 (estimated) | Cousins and Mackay (2000) |
| Aerobic ready biodegradation in water | 42−98% in 28 days | BASF (2007b)<br>BASF (2007a)<br>EC/HC (2015a) |
| Aerobic biodegradation in sediment (DBP as analog) | $t_{1/2}$ = 2.9 days in natural river sediment collected from the Zhonggang, Keya, Erren, Gaoping, Donggang, and Danshui Rivers, Taiwan. | Yuan et al. (2002) |
| Anaerobic biodegradation in sediment | 0 to 30% after 56 days in marine sediment. | NCBI (2020) |
| Aerobic biodegradation in soil | 88.1−97.2% after 200 days in | Inman et al. (1984) |

| Parameter | Selected Value(s) | Reference(s) |
|---|---|---|
| (DBP as analog) | Chalmers slit loam, Plainfield sand, and Fincastle silt loam soils. | |
| Hydrolysis | Rate constant at pH 10−12: 1.4E−03 $M^{-1}$ $s^{-1}$ | Wolfe et al. (1980) |
| | $t_{1/2}$ at pH 7: 5.3 years at 25°C (estimated);<br>$t_{1/2}$ at pH 8: 195 days at 25°C (estimated) | U.S. EPA (2017) |
| Photolysis | Direct: Expected to be susceptible to direct photolysis by sunlight; contains chromophores that absorb at wavelengths >290 nm | NLM (2013) |
| | Indirect: $t_{1/2}$ = 1.15 days (27.6 hours) (estimated; based on a 12-hour day with 1.5E06 ·OH/$cm^3$ and ·OH rate constant of 9.26E−12 ·OH/$cm^3$ and ·OH $cm^3$/molecule-sec) | U.S. EPA (2017) |
| Environmental degradation half-lives<br>(selected values for modeling) | 27.6 hours (air)<br>5 days (water)<br>10 days (soil)<br>45 days (sediment) | U.S. EPA (2017) |
| WWTP Removal | 65−95% | U.S. EPA (1982)<br>Tran et al. (2014) |
| Aquatic Bioconcentration (BCF) | 30.2 L/kg wet weight (upper trophic Arnot-Gobas estimation) | U.S. EPA (2017) |
| Aquatic Bioaccumulation (BAF) | 30.2 L/kg wet weight (upper trophic Arnot-Gobas estimation) | U.S. EPA (2017) |
| Aquatic Food web Magnification Factor (FWMF) | Food-web magnification factor (FWMF): 0.81 (Experimental; 18 marine species) | Mackintosh et al. (2004) |
| Terr. Bioconcentration (BCF) | BCF: 2.23 at 0.13 mg/kg in onion, celery, pepper, tomato, bitter gourd, eggplant, and long podded cowpea. | Li et al. (2016) |
| Terr. Biota-sediment accumulation factor (BSAF) (DBP as analog) | 0.18−0.460 (*Eisenia fetida*) | Hu et al. (2005)<br>Ji and Deng (2016) |

## 3.1 Tier I Analysis

To be able to understand and predict the behaviors and effects of DIBP in the environment, a Tier I analysis will determine whether an environmental compartment (*e.g.*, air, water, etc.) will accumulate DIBP at concentrations that may lead to risk (*i.e.*, major compartment) or are unlikely to result in risk (*i.e.*, minor compartment). The first step in identifying the major and minor compartments for DIBP is to consider partitioning values (Table 3-1) which indicate the potential for a substance to favor one compartment over another. DIBP does not naturally occur in the environment; however, DIBP has been detected in water, soil, and sediment in environmental monitoring studies (EC/HC, 2015a; NLM, 2013).

### 3.1.1 Soil, Sediment, and Biosolids

Based on the partitioning values shown in Table 3-1, DIBP will favor organic carbon over water or air. Because organic carbon is present in soil, biosolids, and sediment, they all are considered major compartments for DIBP. This is consistent with monitoring data from the Mersey River, Liverpool, UK where higher concentrations of DIBP were detected in sediment samples (33.2−93.82 ng/g) compared to water samples (0.338−1.1 ug/L) (Preston and Al-Omran, 1989).

### 3.1.2 Air

DIBP is a liquid at environmental temperatures with a melting point of -64°C and a vapor pressure of $4.76\times10^{-5}$ mm Hg at 25°C (NLM, 2013). DIBP will exist predominantly in the particulate phase with potential to exist in the vapor (gaseous) phase in the atmosphere (EC/HC, 2015a). The octanol:air coefficient ($K_{OA}$) (log value of 9.47 (U.S. EPA, 2017)) indicates that DIBP will favor the organic carbon present in airborne particles. Based on its physical and chemical properties and short half-life in the atmosphere ($t_{1/2}$ = 1.15 days (U.S. EPA, 2017)), DIBP was assumed to not be persistent in the air. The AEROWINTM module in EPI SuiteTM estimates that a small fraction of DIBP could be sorbed to airborne particulates and these particulates may be resistant to atmospheric oxidation. DIBP has been detected in both outdoor air (EC/HC, 2015a; NLM, 2013) and settled house dust (Kubwabo et al., 2013; NLM, 2013; Wang et al., 2013).

### 3.1.3 Water

The air:water partitioning coefficient ($K_{AW}$) (log values of -4.27 and -4.3 (Lu, 2009; Cousins and Mackay, 2000)) indicates that DIBP will favor water over air. DIBP is expected to be slightly soluble in water with a water solubility of 6.2 mg/L at 24°C (NLM, 2013). In water, DIBP will partition to suspended organic material present in the water column based on DIBP's low water solubility and high partition coefficient to organic matter. This is consistent with measured data from False Creek seawater showing concentrations of DIBP ranging from 3 to 9 ng/L (total) with the dissolved fraction concentrations ranging from 2 to 6.7 ng/L and the suspended particulate fraction concentration ranging from 532 to 2,650 ng/g dry weight (dw) (Mackintosh et al., 2006). Although DIBP has low water solubility, surface water will be considered a major compartment for DIBP since DIBP is detected in the ng/L range in water.

## 3.2 Tier II Analysis

A Tier II analysis involves reviewing environmental release information for DIBP to determine whether further assessment is warranted for each environmental medium. Environmental release data for DIBP was not available from the Toxics Release Inventory (TRI) or Discharge Monitoring Reports (DMRs), therefore DIBP releases to the environment could not be estimated. However, between 385,000 and 441,000 pounds of DIBP were produced annually from 2016 to 2019 for use in commercial products, chemical substances or mixtures sold to consumers, or at industrial sites, according to production data from the Chemical Data Reporting (CDR) 2020 reporting period. DIBP is used in adhesives and sealants, electrical/electronics, children's toys and articles, and plastic and rubber materials. DIBP is not chemically bound to the polymer matrix and can migrate from the surface of polymer products (EC/HC, 2015b). Therefore, DIBP can easily leach or diffuse into the surrounding environment during the production, usage, and disposal of polymer products. Additionally, DIBP may be released to the environment from disposal of wastewater, and liquid and solid wastes. After undergoing wastewater treatment processes, the disposal of wastewater or liquid wastes results in effluent discharge to water and land application of biosolids, which would lead to media specific evaluations (Table 3-2). Releases from landfills and incinerators will occur from the disposal of liquid and solid wastes and warrants media specific evaluations.

**Table 3-2. Summary of Key Environmental Pathways and Media Specific Evaluations**

| Environmental Releases | Key Pathway | Media Specific Evaluations |
|---|---|---|
| Wastewater and liquid waste treatment | Effluent discharge to water and land application of biosolids | Air, water, sediment, soil, groundwater, and biosolids |
| Disposal of liquids and solids to landfills | Leachate discharge to water and biogas to air | Air, water sediment, soil, and groundwater |
| Incineration of liquid and solids | Stack emissions to air and ash to landfill | Air, water, sediment, soil, and groundwater |
| Urban/remote areas | Fugitive emissions to air | Air, water, sediment, soil, and groundwater |
| | Deposition | Water and soil |
| | Partitioning | Water, sediment, soil, and groundwater |

### 3.2.1 Fugacity Modeling

The approach described by Mackay (1996) using the Level III Fugacity model in EPI Suite™ (V4.11) (LEV3EPI™) was used for this Tier II analysis. LEV3EPI is described as a steady-state, non-equilibrium model that uses a chemical's physical and chemical properties and degradation rates to predict partitioning of the chemical between environmental compartments and its persistence in a model environment (U.S. EPA, 2017).

The following input parameters were used for the Level III Fugacity model in EPI Suite™:

- Melting Point = -64.00 ºC
- Vapor Pressure = $4.76\times10^{-5}$ mm Hg
- Water Solubility = 6.2 mg/L
- Log $K_{OW}$ = 4.34
- SMILES: O=C(OCC(C)C)c(c(ccc1)C(=O)OCC(C)C)c1 (representative structure)

DIBP's physical and chemical properties were taken directly from Section 2.1. Environmental degradation half-lives for DIBP and DBP (as analog) were taken from high and medium quality studies that were identified through systematic review to use information from the best available source, fill data gaps, and help reduce the levels of uncertainties. The environmental degradation half-life in water of five days was selected to represent the range of identified primary biodegradation half-life values (Section 4.1) from high and medium quality studies to reduce levels of uncertainties. The EPA used environmental degradation half-lives of 27.6 hours in air (based on AEROWIN™ predicted values, an atmospheric fate prediction model within EPI Suite™), 10 days in soil (double the half-life in water), and 45 days in sediment (nine times the half-life in water) as recommended for EPIWIN estimations (U.S. EPA, 2017). The Level III Fugacity model estimated DIBP's overall environmental half-life of 5 days (100% DIBP released to air), 7 days (100% DIBP released to water), 14 days (100% DIBP released to soil), and 9 days (equal release of DIBP to air, water, and soil). For this *Risk Evaluation* EPA selected an overall environmental half-life of 14 days for DIBP.

Based on DIBP's environmental half-lives, partitioning characteristics, and the results of Level III Fugacity modeling, DIBP is expected to be found predominantly in water, soil, and air (Figure 3-1). DIBP is expected to partition primarily to soil from releases to air, or in scenarios of direct soil release. Releases to soil are expected to remain in soil while releases to water are expected to remain primarily in water with a small fraction partitioning to sediments. The LEV3EPI™ results were consistent with environmental monitoring data. Further discussion of DIBP media specific assessment can be found in Section 5.

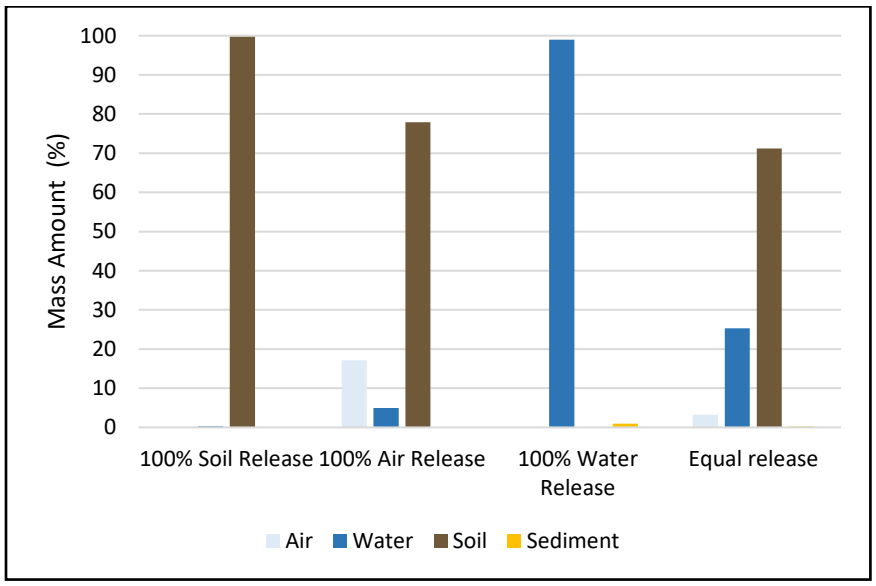


**Figure 3-1. EPI SuiteTM Level III Fugacity Modeling Graphical Result for DIBP**

# 4 TRANSFORMATION PROCESSES

DIBP released to the environment is expected to transform to the monoester form (monoisobutyl phthalate) via abiotic processes such as photolysis (direct and indirect) and hydrolysis of the carboxylic acid ester group (U.S. EPA, 2023). Biodegradation pathways for the phthalates consist of primary biodegradation from phthalate diesters to phthalate monoesters, then to phthalic acid, and ultimately biodegradation of phthalic acid to form $CO_2$ and/or $CH_4$ (Huang et al., 2013). Monoisobutyl phthalate is both more soluble and more bioavailable than DIBP. It is also expected to undergo biodegradation more rapidly than the diester form. EPA considered DIBP transformation products qualitatively but due to their lack of persistence we do not expect them to substantially contribute to risk, thus EPA is not considering them further in this risk evaluation. Both biotic and abiotic routes of degradation for DIBP are described in the sections below.

## 4.1 Biodegradation

DIBP can be considered readily biodegradable in most aquatic environments with extended half-lives in soils and anaerobic environmental compartments. The EPA extracted and evaluated seven data sources containing DIBP biodegradation information in water and sediments under aerobic and anaerobic conditions and two data sources containing DBP (as DIBP analog) soil and sediment biodegradation information (Table 4-1). Three of the DIBP data sources were classified as overall high-quality and four as overall medium-quality data sources. The two DBP data sources were classified and extracted as overall high-quality. Several ready biodegradability tests have reported DIBP's aerobic biodegradation in water to be 40 to 98 percent in 28 days (NCBI, 2020; EC/HC, 2015a; Harlan Laboratories, 2010; BASF, 2007a, b). Except for one study, all the studies indicate DIBP is readily biodegradable. A river die-away test estimated a half-life of 0.87 days for DIBP (NCBI, 2020). Other studies evaluating the biodegradability of DIBP have measured biodegradation of 15 percent in 7 days and 35 percent in 14 days in seawater (NCBI, 2020), as well as 100 percent in 7 days in river water (Hashizume et al., 2002). The available data suggest that DIBP is expected to biodegrade rapidly in most aerobic environments.

In contrast, DIBP it is expected to have low biodegradation potential under low oxygen conditions and may be expected to persist in subsurface sediments. One study measured 0 to 30 percent biodegradation under anaerobic conditions in swamp water over 96 days (NCBI, 2020). The biodegradation of DBP (DIBP isomer) has been reported to be 88.1 to 97.2 percent loss of parent substance after 200 days in soils and to have a half-life of 2.9 days in natural river sediments (Yuan et al., 2002; Inman et al., 1984). In general, DIBP is expected to readily biodegrade under most environmental conditions and is expected to persist for extended periods of time in anaerobic environmental compartments.

**Table 4-1. Summary of DIBP's Biodegradation Information**

| Property | Selected Value(s) | Reference(s) | Data Quality Rating |
|---|---|---|---|
| Aerobic primary biodegradation in water: Removal | 100% in 6 days | Hashizume et al. (2002) | Medium |
| | 98% in 28 days | SRC (1984)<br>EC/HC (2015a) | Medium |
| | 66−70% in 28 days. | BASF (2007a) | High |
| | 60−70% and 70−80% in 28 days | EC/HC (2015a) | Medium |
| | 42% in 28 days | EC/HC (2015a) | Medium |
| | 80% in 28 days | BASF (2007b) | High |

| Property | Selected Value(s) | Reference(s) | Data Quality Rating |
|---|---|---|---|
| | 40% in 28 days | Harlan Laboratories (2010) | High |
| | 60−70% in 28 days. | EC/HC (2015a) | Medium |
| Aerobic primary biodegradation in seawater: Removal | 15% in 7 days | NCBI (2020) | Medium |
| | 35% in 14 days | NCBI (2020) | Medium |
| Aerobic primary biodegradation in seawater: Half-life | $t_{1/2}$ = 0.87 days | NCBI (2020) | Medium |
| Aerobic biodegradation in sediment: Half-life (DBP as analog) | $t_{1/2}$ = 2.9 days | Yuan et al. (2002) | High |
| Anaerobic biodegradation in sediment: Removal | 0−30% in 96 days | NCBI (2020) | Medium |
| Aerobic biodegradation in soil: Removal (DBP as analog) | 88.1−97.2% after 200 days | Inman et al. (1984) | High |

## 4.2 Hydrolysis

EPA did not identify abiotic hydrolysis data for DIBP collected by applicable, accepted test methods (*e.g.*, OECD Guideline Test 111) through the systematic literature review process. Wolfe (1980) evaluated the hydrolysis of DIBP in aqueous alkaline solutions at 30 °C. The study reported hydrolysis to be very slow under the tested conditions reporting a second order hydrolysis rate constant of $1.40\times10^{-03}$ $M^{-1}*s^{-1}$ for DIBP. This finding suggests DIBP to have a hydrolysis half-life greater than 2 years in water at pH 10 to 12 and 30 °C, and hydrolysis is less likely to occur under environmental conditions. In addition, EPI Suite™ estimated the hydrolysis half-lives of DIBP at 5.3 years at pH 7 and 25 ºC, and 195 days at pH 8 and 25 ºC (U.S. EPA, 2017) indicating that hydrolysis of DIBP is more likely under more caustic conditions and is unlikely under normal environmental conditions.

When compared to other degradation pathways, hydrolysis it is not expected to be a significant source of degradation under typical environmental conditions. Like other phthalate esters, the higher temperatures, variations from typical environmental pH, and chemical catalysts present in the deeper anoxic zones of landfills may be favorable to the degradation of DIBP via hydrolysis (Huang et al., 2013). This is discussed further in Section 5.3.3.

## 4.3 Photolysis

DIBP contains chromophores that absorb light at greater than 290 nm wavelength (NLM, 2013), therefore, direct photodegradation is a relevant degradation pathway for DIBP released to air. Modelled indirect photodegradation half-lives indicate a slightly more rapid rate of degradation than direct photodegradation, estimating a half-life of 1.15 days (27.6 hours) (·OH rate constant of $9.26\times10^{-12}$ $cm^3$ /molecule-second and a 12-hour day with $1.5\times10^6$ $OH/cm^3$) (U.S. EPA, 2017). Similarly, Peterson (2003) reported a calculated DIBP photodegradation half-life of 0.89 days (21.4 hours) (·OH rate constant of $9.26\times10^{-12}$ $cm^3$ /molecule-second and $1\times10^6$ $OH/cm^3$).

DIBP photodegradation in water is expected to be slower than air, due to the typical light attenuation in natural surface water. There is limited information on the aquatic photodegradation of DIBP. However, Lertsirisopon (2009) reported DBP (DIBP isomer) aquatic direct photodegradation observed half-lives of 50, 66, 360, 94 and 57 days at pH 5, 6, 7, 8 and 9, respectively, when exposed to natural sunlight in artificial river water at 0.4 to 27.4°C (average temperature of 10.8°C). These findings suggest that DIBP is susceptible to photochemical decay in atmospheric air but that photochemical decay is not expected to be a significant degradation process in surface water.

# 5 MEDIA ASSESSMENTS

DIBP has been reported to be present in the atmosphere, aquatic environments, and terrestrial environments. Once in the air, DIBP will be most predominant in the organic matter present in airborne particles and is expected to have a short half-life in the atmosphere. Based on the physical and chemical properties, DIBP is likely to partition to house dust and airborne particles in the indoor environment, and is expected to have a longer half-life indoors as compared to ambient (outdoor) air. Once in water, the Level III Fugacity Model in EPI Suite™ (U.S. EPA, 2017) predicts that close to 99 percent of the DIBP will remain in water (Section 3.2). However, DIBP is expected to readily biodegrade in most aquatic environments (BASF, 2007a, b). In addition, the available data sources suggest that DIBP present in surface water to potentially have higher than predicted partitioning to aquatic sediments and suspended organic matter. DIBP is expected to have an aerobic biodegradation half-life of 5 days. In terrestrial environments DIBP has the potential to be present in soils and ground water, is likely to be more mobile in groundwater than higher molecular weight PAEs, but is not likely to be persistent in groundwater/subsurface environments unless anoxic conditions exist (4.1). In soils, DIBP is expected to be deposited via air deposition and land application of biosolids. DIBP in soils is expected to have a half-life on the order of days to weeks (based on the estimated half-life of 10 days), and have low bioaccumulation potential and biomagnification potential in terrestrial organisms. DIBP is released to groundwater via wastewater effluent and landfill leachates, is expected to have a half-life of 14 days, and is not likely to be persistent in most groundwater/subsurface environments.

## 5.1 Air and Atmosphere

DIBP is a liquid at environmental temperatures with a melting point of -64°C (Haynes, 2014) (NLM, 2013) and a vapor pressure of $4.76\times10^{-5}$ mmHg at 25°C (NLM, 2013). Based on its physical and chemical properties and short half-life in the atmosphere, $t_{1/2}$ = 27.6 hours (U.S. EPA, 2017), DIBP was assumed to not be persistent in the air. The AEROWIN™ module in EPI Suite™ estimated that DIBP present in air is likely to be sorbed to airborne particles and these particulates may be resistant to atmospheric oxidation. Available data sources have reported DIBP to be detected in air gas phase at concentrations of 0.250, 8.5 to 515.8, and 1682 to 2038 ng/m$^3$ in the Artic, China, and India, respectively (Net et al., 2015; Das et al., 2014). However, based on DIBP's short half-life in the atmosphere, it is not expected to be persistent in atmospheric air under normal environmental conditions.

### 5.1.1 Indoor Air and Dust

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 DEHP (diethylhexyl phthalate) to be the predominant phthalate ester in the environment. However, the available data sources reported DIBP to be present at higher concentrations in air phase than DEHP (Net et al., 2015) and to be found in air at higher concentrations indoors than outdoors (Das et al., 2014; Wormuth et al., 2006). In addition, the available information suggests that DIBP released to air preferentially accumulated in suspended particles and dust (Das et al., 2014; Kanazawa et al., 2010; Wormuth et al., 2006). These findings are supported by the LEV3EPI predicted partitioning during a DIBP release to air scenario. The LEV3EPI predicted 77.9 percent DIBP in air to partition to organic matter in soil, 4.94 percent to water, and 17.1 percent to remain suspended in air (U.S. EPA, 2017). DIBP is expected to be more persistent in indoor air than in ambient (outdoor) air due to the lack of natural chemical removal processes indoors, such as solar photochemical degradation.

The EPA identified several data sources reporting the presence of DIBP in indoor settings. The available data sources have reported the presence of DIBP in indoor air and dust. In general, these studies reported higher concentration of DIBP in dust than air. For instance, Kanazawa (2010) collected air room

samples from 40 dwellings in Sapporo, Japan. In the study DIBP was detected in all indoor air and dust samples with median concentrations of 75 ng/m$^3$, and 2.4 mg/kg, respectively. In a similar study, Wormuth (2006) determined the indoor air and indoor dust concentrations of DIBP, DBP, BBP, and DEHP based on measured concentrations of phthalates in dust of European homes. The study reported DIBP mean indoor air concentrations of 86 ng/m$^3$ and mean indoor dust concentrations of 84 mg/kg. In addition, the available data suggest that the introduction of household products containing DIBP and the proximity to industrial activities related to their use and production to potentially increase the concentration of DIBP in indoor air and dust. Das (2014) explored the implications of industrial activities by comparing the presence of phthalates in two different cities from India. The study analyzed indoor air and dust samples from JNU (a city with low industrial activities) and Okhla (a city with high industrial activities related to the use of phthalates), reporting a general tendency of higher detectable concentrations of DIBP, DBP, BBP, DCHP, and DEHP in air and dust samples collected in the city of Okhla. This finding suggests that higher concentrations of phthalates in air and dust could be expected near facilities with high use and production of phthalates. In the US, the available data reported DIBP indoor dust concentrations of 12 mg/kg (CA), 1.32 mg/kg (Philadelphia, MA), and 4.367 mg/kg (Durham, NC) (Hammel et al., 2019; Dodson et al., 2015; Rudel et al., 2001). Dodson (2017) evaluated the presence of phthalate esters in air samples of US homes before and after occupancy reporting a general increased presence of phthalates after occupancy due to daily anthropogenic activities that might introduce phthalate containing products into indoor settings. Increasing trends could be expected for DIBP with its increased use in household construction materials and consumer products.

## 5.2 Aquatic Environments

### 5.2.1 Surface Water

DIBP is expected to be released to surface water via industrial and municipal wastewater treatment plant effluent, surface water runoff, and, to a lesser degree, atmospheric deposition. DIBP has frequently been detected in surface waters in the µg/L to mg/L range (Zeng et al., 2008; Wang et al., 2005; Tan, 1995; Preston and Al-Omran, 1989). The principal properties governing the fate and transport of DIBP in surface water are water solubility (6.2 mg/L), air:water partitioning coefficient (log $K_{AW}$ = -4.3), and organic carbon:water partitioning coefficient (log $K_{OC}$ = 2.67). Due to the Henry's law constant of DIBP ($1.83\times10^{-7}$ atm·m$^3$/mol at 25 °C), volatilization is not expected to be a significant source of loss of DIBP from surface water.

A partitioning analysis of a continuous release of DIBP to water estimates that once steady state has been reached about 1 percent of DIBP will partition to sediments and about 99 percent will remain in surface water as described in Section 3.2.1 above. However, several data sources have documented the presence of DIBP in sediments and suspended solids to be higher than in water (Section 5.2.2). In addition, based on the organic carbon:water partition coefficient (log $K_{OC}$ = 2.67), DIBP in water is expected to partition to suspended particles and sediments. The available data sources reported the presence of DIBP and other phthalates in surface water samples collected from rivers and lakes. Peterson and Al-Omran (1989) explored the presence of phthalates within the River Mersey Estuary reporting the presence of DIBP freely dissolved in the water phase at concentrations of 0.338 to 1.100 µg/L. While Tan (1995) did not detect DIBP in the Klang River in all samples collected, DIBP concentrations up to 3.3 µg/L were reported from samples where DIBP was detected. Zeng et al. (2008) reported the presence of DIBP in the dissolved aqueous phase of urban lakes in Guangzhou City at a mean concentration of 0.47 µg/L. Grigoriadou et al. (2008) reported the presence of DIBP in lake water samples collected near the industrial area of Kavala city. The detected DIBP concentration range in lake water was reported to be 0.067 to 3.800 µg/L. False Creek seawater concentrations of DIBP ranged from 3 to 9 ng/L (total) with the dissolved fraction concentrations ranging from 2 to 6.7 ng/L and the

suspended particulate fraction concentration ranging from 532 to 2,650 ng/g dry weight (dw) (Mackintosh et al., 2006). The available information suggests DIBP to potentially be found in high frequency in surface water with higher concentrations in sediments and suspended particles (Grigoriadou et al., 2008; Preston and Al-Omran, 1989). However, DIBP is expected to be readily biodegradable, not persistent, and to have a half-life of five days in surface water (Section 4.1 and Table 3-1).

### 5.2.2 Sediments

Based on the expected sorption of DIBP to organic matter, DIBP will partition to the organic matter present in soils and sediment when released into aquatic environments. Once in water, the Level III Fugacity Model in EPI Suite™ (U.S. EPA, 2017) predicts that close to 99 percent of the DIBP will remain in water (Section 3.2.1). However, DIBP is expected to readily biodegrade in most aquatic environments (BASF, 2007a, b). The available data sources indicate that phthalate esters classified as inherently biodegradable in sediments could potentially persist longer with increasing sorption potential to sediments (Kickham et al., 2012). This suggests that DIBP could persist longer in subsurface sediments and soils than in water, to have the potential to accumulate in sediments at areas of continuous release, such as a surface water body receiving discharge from a municipal wastewater treatment plant.

Due to the strong sorption to organic carbon (log $K_{OC}$ = 2.67), DIBP in water is expected to be found predominantly in sediments near point sources. This is consistent with available monitoring data showing presence of DIBP in river, lake, and marine sediment samples. Recent studies have reported the presence of DIBP in river sediment samples at concentrations between 1.2 and 866.67 ng/g dw (Cheng et al., 2019; Li et al., 2017b; Li et al., 2017a; Tang et al., 2017; Tan, 1995; Preston and Al-Omran, 1989). Similar and higher concentrations of DIBP in sediments have been reported in samples from lakes in Guangzhou and Beijing (Zheng et al., 2014; Zeng et al., 2008). Zheng (2014) reported a direct relationship between the detection of DIBP in sediment and anthropogenic activities. The study reported the presence of DIBP in sediment samples collected from the Guanting Reservoir, the Lakes Shichahai and the Lakes in Summer Palace in Beijing at a mean concentration range of 118.1 to 338.0 ng/g dw. In a similar study, Zeng et al. (2008) explore the presence of phthalate esters in urban lakes in a subtropical city of Guangzhou, reporting a mean concentration of DIBP in sediment of 16.010 µg/g dw. Saeed et al. (2017) reported the presence of DIBP in marine sediment samples from the Kuwait coastal areas receiving sewage effluents. The study reported DIBP average concentration in sediment of 243.18 ng/g dw. Mackintosh et al. (2006) reported higher concentrations of DIBP in the suspended particles than in deep sediment of samples collected from the False Creek Harbor in Vancouver. The study reported DIBP mean concentrations of 4 and 1,190 ng/g in the deep sediment and suspended particles, respectively. In a similar study, Kim et al. (2021) evaluated the presence of plasticizers in sediments from highly industrialized bays of Korea. DIBP was detected in 90 percent of the collected surface sediment samples at a median concentration of 0.90 ng/g dw. The study revealed a gradual decreasing trend in the overall concentration of phthalates toward the outer region of the bays farther away from industrial activities. The findings of this study suggest industrial activities to be the major contributor of phthalates in sediments within the area.

## 5.3 Terrestrial Environment

### 5.3.1 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). Typically, chemical substances with very low water solubility and high sorption potential are

expected to be sorbed to suspended solids and efficiently removed from wastewater via accumulation in sewage sludge and biosolids.

As described in Section 6.2, DIBP in wastewater has been reported to be mainly removed by particle sorption and retained in the sewage sludge. Based on EPI Suite™ STP module, about 15 percent of DIBP present in wastewater is expected to accumulate in sewage sludge and biosolids. Three studies have reported DIBP's concentration in sludge in Chinese WWTPs to be 0.0003 to 5.92 µg/g dw (Zhu et al., 2019; Meng et al., 2014) and 0.074 to 7.5 µg/g dw in 40 Korean WWTPs (Lee et al., 2019). Two other studies report sludge concentrations in the United States of 0.32 to 17 µg/g (Howie, 1991) and 966 µg/L (ATSDR, 1999). Once in biosolids, DIBP could be transferred to soil during land applications.

### 5.3.2 Soil

DIBP is expected to be deposited to soil via two primary routes: application of biosolids and sewage sludge in agricultural applications or sludge drying applications; and atmospheric deposition. Based on DIBP's Henry's Law constant of $1.83\times10^{-7}$ atm·m$^3$/mol at 25 °C and vapor pressure of $4.76\times10^{-5}$ mm Hg, DIBP is not likely to volatilize from soils. DIBP shows a moderate affinity for sorption to soil and its organic constituents (log Koc = 2.67 and log $K_{OW}$ = 4.34 (Table 3-1)). Given that these properties indicate the likelihood of moderate sorption to organic carbon present in soil, DIBP is expected to have moderate mobility in soil environments.

DIBP will sorb to organic matter in soils with a predicted overall environmental persistence of 14 days when released to soil (Section 3.2.1). DIBP is expected to be more persistent in soil profiles with anaerobic conditions (NCBI, 2020). Despite its sorption to soils, DIBP present in soils is expected to be moderately mobile in the environment and terrestrial organisms may be exposed to DIBP via this pathway. However, terrestrial species have been reported to have the capacity to metabolize phthalate substances (Bradlee and Thomas, 2003; Gobas et al., 2003; Barron et al., 1995) and DIBP is expected to have low bioaccumulation potential and biomagnification potential in terrestrial organisms (Section 7).

Under aerobic conditions, a half-life in soil of 10 days is estimated for DIBP. This aerobic biodegradation half-life for soil was estimated by doubling the experimentally derived half-life of DIBP in water as very limited soil biodegradation data for DIBP was identified in the systematic review process as described in Section 4.1 (SRC, 1983). The results from EPISuite™ suggest that DIBP will not degrade rapidly in anaerobic environments. This is supported by NCBI (2020) which reports 0 to 30 percent biodegradation in 96 days in anaerobic sediments.

In general, DIBP is not expected to be persistent in soil as long as the rate of release does not exceed the rate at which biodegradation can occur, but continuous exposure to DIBP in soil proximal to points of release may be possible if the rate of release exceeds the rate of biodegradation under aerobic conditions. Under anaerobic conditions in soil, DIBP is assumed to be persistent, and continuous exposure is likely.

### 5.3.3 Landfills

For the purpose of this assessment, landfills will be considered to be divided into two zones: an "upper-landfill" zone, with normal environmental temperatures and pressures, where biotic processes are the predominant route of degradation for DIBP, and a "lower-landfill" zone where elevated temperatures and pressures exist, and abiotic degradation is the predominant route of degradation for DIBP. In the upper-landfill zone where oxygen may still be present in the subsurface, conditions may still be favorable for aerobic biodegradation, however, photolysis and hydrolysis are not considered to be significant sources of degradation in this zone. In the lower-landfill zone, conditions are assumed to be

anoxic, and temperatures present in this zone are likely to inhibit biotic degradation of DIBP. In lower-landfills, there is some evidence to support that hydrolysis may be the main route of abiotic degradation of phthalate esters (Huang et al., 2013). Temperatures in lower-landfills may be as high as 70 ºC. At temperatures at and above 60 ºC, biotic processes are significantly inhibited, and are likely to be completely irrelevant at 70 ºC (Huang et al., 2013).

DIBP is deposited in landfills continually and in high amounts from the disposal of consumer products containing DIBP. Similar to other phthalate esters, under anaerobic conditions present in lower-landfills, DIBP is likely to be persistent due to the expected negligible biodegradation potential. Some aerobic biodegradation may occur in upper-landfills. Due to the expected persistence of DIBP in landfills, it may dissolve into leachate in small amounts based on a water solubility of 6.2 mg/L and may travel slowly to ground water during infiltration of rainwater based on a low log Koc of 2.67. DIBP has been reported in landfill leachates at concentrations of 11.67 µg/L, 0.1 µg/L, 3.43 µg/L in China, USA, and Poland, respectively (Kotowska et al., 2020; Liu et al., 2010; CEC, 1976). In addition, DIBP has been detected in surface water and groundwater downstream of landfills at concentrations of 0.40 µg/L and 3.41 µg/L, respectively (Liu et al., 2010). In lower-landfills, there is some evidence to support that hydrolysis may be the main route of abiotic degradation of phthalate esters (Huang et al., 2013).

### 5.3.4 Groundwater

There are several potential sources of DIBP in groundwater, including wastewater effluents and landfill leachates, which are discussed in Sections 6.2 and 5.3.3. Further, in environments where DIBP is found in surface water, it may enter groundwater through surface water/groundwater interactions. Diffuse sources include storm water runoff and runoff from biosolids applied to agricultural land.

Given the strong affinity of DIBP to adsorb to organic matter present in soils and sediments (log Koc = 2.67) (He et al., 2019), DIBP is expected to have low mobility in soil. However, due to DIBP's water solubility (6.2 mg/L), DIBP partitioning to groundwater environments is possible resulting in small concentrations of DIBP in groundwater. For instance, the concentration of DIBP in groundwater has been reported to be 0.237 µg/L, 0.1 µg/L, and 0.655 µg/L in China, USA, and France, respectively (Bach et al., 2020; NCBI, 2020; Dong et al., 2018). In instances where DIBP could reasonably be expected to be present in groundwater environments (proximal to landfills or agricultural land with a history of land applied biosolids), limited persistence is expected based on rates of biodegradation of DIBP in aerobic environments (Section 4.1), DIBP is not likely to be persistent in groundwater/subsurface environments unless anoxic conditions exist.

# 6 REMOVAL AND PERSISTENCE POTENTIAL OF DIBP

DIBP is not expected to be persistent in the environment, as it is expected to degrade rapidly under most environmental conditions, with delayed biodegradation in low-oxygen media. In the atmosphere, DIBP 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 27.6 hours. DIBP is predicted to hydrolyze slowly at ambient temperature, but is not expected to persist in aquatic media as it undergoes rapid aerobic biodegradation (Section 5.2.1). DIBP has the potential to remain for longer periods of time in soil and sediments, and due to its sorption potential (log Koc = 2.67) DIBP uptake by aquatic organisms is possible. However, terrestrial species have been reported to have the capacity to metabolize phthalate ester substances (Bradlee and Thomas, 2003; Gobas et al., 2003; Barron et al., 1995). Using the Level III Fugacity model in EPI Suite™ (LEV3EPITM) (Section 3.2.1), DIBP's overall environmental persistence was estimated to be approximately 14 days (U.S. EPA, 2017). Therefore, DIBP is not expected to be persistent in the atmosphere or aquatic and terrestrial environments.

## 6.1 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. DIBP is classified as a hazardous substance and 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) (U.S. EPA, 1981).

Currently there is no information available on the DRE of DIBP. However, the DEHP annual releases from a Danish waste incineration facility were estimated to be 9 percent to air and 91 percent to municipal land fill (ECB, 2008). These results suggest that DIBP present during incineration processes will mainly be released to landfills, with a small fraction released to air. Based on its water solubility and sorption potential, DIBP released to landfills is expected to partition to waste organic matter. Similarly, DIBP released to air is expected to rapidly react via indirect photochemical processes within hours (U.S. EPA, 2017) and partition to soil and water as described in Section 3.2.1. DIBP in sediments and soils is not expected to be bioavailable for uptake and is highly biodegradable in its bioavailable form (Kickham et al., 2012).

## 6.2 Removal in Wastewater Treatment

Wastewater treatment is performed to remove contaminants from wastewater using physical, biological, and chemical processes. Generally, municipal wastewater treatment facilities apply primary and secondary treatments. During the primary treatment, screens, grit chambers, and settling tanks are used to remove solids from wastewater. After undergoing primary treatment, the wastewater undergoes a secondary treatment. Secondary treatment processes can remove up to 90 percent of the organic matter in wastewater using biological treatment processes such as trickling filters or activated sludge. Sometimes an additional stage of treatment such as tertiary treatment is utilized to further clean water for additional protection using advanced treatment techniques (*e.g.*, ozonation, chlorination, disinfection) (U.S. EPA, 1998).

Limited information is available on the fate and transport of DIBP in wastewater treatment systems. The EPA selected four data sources (3 rated as high quality and 1 rated as medium quality) reporting the removal of DIBP in wastewater treatment systems employing both aerobic and anaerobic processes. The available data sources reported 31 to 98 percent removal of DIBP from WWTP effluents (Table 6-1). One study reported 96.7 percent DIBP removal efficiencies in a municipal wastewater treatment facility

in France, employing a combined decantation and activated sludge tank. DIBP was reported to be mainly removed by particle sorption and retained in the sewage sludge (Tran et al., 2014). Similarly, Peterson (2003) reported 98 percent removal of DIBP from the effluent of two WWTPs treating domestic and industrial wastewater. These findings agree with the STPWIN predicted DIBP removal of 95 percent in domestic wastewater treatment systems (U.S. EPA, 2017). In addition, the median removal of DBP (DIBP analog) has been reported to be 68 to 98 percent within 50 WWTPs in the U.S. (U.S. EPA, 1982). However, DIBP has been reported to be removed by 65 percent and -26 to 59 percent removal in WWTPs from Sweden and Hong Kong, respectively (NCBI, 2020; Wu et al., 2017).

Unlike other phthalates esters with longer carbon chains, DIBPs slight water solubility (6 mg/l) and relatively lower log Koc (2.67) suggests partial removal via sorption to sludge. This finding is supported by STPWIN™, by the predicted 35 percent removal of DIBP during conventional wastewater treatment by sorption to sludge with the potential of increased removal via rapid aerobic biodegradation processes (U.S. EPA, 2017). Similarly, a study of WWTPs in Korea reported average emission fluxes of DIBP of 10.6 kg/day/WWTP in sludge and 19.8 kg/day/WWTP in the treated effluent (Lee et al., 2019). In general, the available information suggest that aerobic processes have the potential to help biodegrade DIBP from wastewater in agreement with the expected aerobic biodegradation described in Section 4.1. However, DIBP may have low removal efficiencies especially in removal processes where biodegradation is not significant. Air stripping within the aeration tanks for activated sludge processing is not expected to be a significant removal mechanism for DIBP present in wastewater removal process. In general, the available DBP information in U.S. WWTPs, the predicted and measured removal of DIBP, WWTPs are expected to remove 65 to 95 percent of DIBP present in wastewater.

**Table 6-1. Summary of DIBP's WWTP Removal Information**

| Property | Selected Value(s) | Reference(s) | Data Quality Rating |
|---|---|---|---|
| Removal (WWTP) | 65% | NCBI (2020) | Medium |
| | 96.7% | Tran et al. (2014) | High |
| | 95% | U.S. EPA (2017) | High |
| | 68−98% (Secondary with AS- DBP as analog) | U.S. EPA (1982) | High |
| Removal (WWTP-Sewage) | 98% | Peterson and Staples (2003) | Medium |
| | 31−39% (primary and secondary without activated sludge)<br><br>59% (primary and secondary with activated sludge) | Wu et al. (2017) | High |

## 6.3 Removal in Drinking Water Treatment

Drinking water in the United States typically comes from surface water (*i.e.*, lakes, rivers, 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 U.S., public water systems often use conventional treatment processes that include coagulation, flocculation, sedimentation, filtration, and disinfection, as required by law.

Limited information is available on the removal of DIBP in drinking water treatment plants. The available data sources reported concentrations of DIBP in drinking water in the range of 0.11 to 1034.7 ng/L (Ding et al., 2019; Li et al., 2019; Kong et al., 2017; Shan et al., 2016; Das et al., 2014; Shi et al., 2012). Kong et al. (2017) explored the presence and removal of phthalate esters in a drinking water treatment system employing coagulation, sedimentation, and filtration treatment processes, and reported 24.3 percent removal of DIBP from the treated effluent. Similarly, Shan et al. (2016) explored the removal of phthalate esters in a drinking water treatment plant employing coagulation, sedimentation, filtration, and disinfection treatment processes and reported 36.2 percent removal of DIBP from the treated effluent. The same data source reported 44.0 percent removal of DIBP from the treated effluent in a second drinking water treatment system employing peroxidation, coagulation, combined flocculation and sedimentation, filtration, and disinfection treatment processes. The slightly higher removal was attributed to the use of ozone preoxidation treatment process. These findings suggest that conventional drinking water treatment systems may have the potential to partially remove DIBP present in drinking water sources via sorption to suspended organic matter and filtering media.

# 7 BIOACCUMULATION POTENTIAL OF DIBP

The presence of DIBP in several marine aquatic species in North America suggests that the substance is bioavailable in aquatic environments (Mackintosh et al., 2004). However, DIBP can be considered readily biodegradable under most aquatic environments and the estimated fish upper trophic level BCF of 30.2 L/kg (U.S. EPA, 2017) and measured log $K_{OW}$ of 4.34 suggest that it is expected to have low bioaccumulation potential. The EPA selected three overall high quality data sources and one overall medium quality data source reporting the aquatic bioconcentration, aquatic bioaccumulation, aquatic food web magnification, and terrestrial bioconcentration of DIBP (Table 7-1).

The available data sources discussed below suggest that DIBP has low bioaccumulation potential in aquatic and terrestrial organisms (Kim et al., 2016; Teil et al., 2012), and no apparent biomagnification across trophic levels in the aquatic food web (Mackintosh et al., 2004). Teil et al. (2012) reported fish aquatic biota-sediment accumulation factors (BSAF) of 62.5±26.5 (Roach), 41.4±13.3 (Chub), and 123.5±75.3 (Perch) samples collected from the Orge River in France. These findings suggest low bioaccumulation potential in aquatic environments, but higher accumulation expected to smaller organisms exposed to DIBP in sediments. However, the reported Trophic Magnification Factor (TMF) of 0.11 and 1.8 and Aquatic Food web Magnification (FWMF) of 0.81 indicates trophic dilution of DIBP from lower to higher trophic levels within the food-web (Kim et al., 2016; Mackintosh et al., 2004).

There is very limited information on the bioconcentration and bioaccumulation of DIBP in terrestrial environments. Based on DIBP's sorption to organic matter (log Koc 2.67) (He et al., 2019) and water solubility (6.2 mg/L) (U.S. EPA, 2019), DIBP is expected to be bioavailable in soils. However, Lua et al. (2016) reported DIBP BCF value of 2.23 on the edible fraction of several fruits and vegetables. This finding suggests low uptake potential of DIBP in soils in edible fruits and vegetables. Therefore, DIBP is expected to have low bioaccumulation potential and low biomagnification potential in terrestrial organisms.

Overall, the available data suggest that DIBP is expected to have low bioaccumulation potential and low biomagnification potential in aquatic and terrestrial organisms.

**Table 7-1. Summary of DIBP's Bioaccumulation Information**

| Property | Selected Value(s) | Reference(s) | Data Quality Rating |
|---|---|---|---|
| Aquatic Bioconcentration (BCF) | 30.2 L/kg<br>Estimated steady-state bioconcentration factor (BCF; L/kg); Arnot-Gobas method, fish upper trophic level. | U.S. EPA (2017) | High |
| Aquatic Biota-sediment accumulation factor (BSAF) | 41.4±13.3 to 123.5 ± 75.3<br>Roach (153 g): 62.5±26.5, Chub (299 g): 41.4±13.3, and Perch (49 g): 123.5±75.3<br>BSAF = $C_{biota}$ (ng/g)/$C_{sediment}$ (ng/g) | Teil et al. (2012) | High |
| Aquatic Trophic Magnification Factor | 0.11−1.8<br>95% confidence interval of the | Kim et al. (2016) | High |

| Property | Selected Value(s) | Reference(s) | Data Quality Rating |
|---|---|---|---|
| (TMF) | reported TMF values in the False Creek food web species including 3 phytoplankton, 1 zooplankton, 10 invertebrates, and 10 fish. | | |
| Aquatic Food web Magnification (FWMF) | 0.81<br>Food-web magnification factor of 0.81 (0.52−1.24) in 18 marine species in the False Creek food web. | Mackintosh et al. (2004) | High |
| Terrestrial Bioconcentration (BCF) | 2.23<br>BCF of edible fraction of onion, celery, pepper, tomato, bitter gourd, eggplant, and long podded cowpea samples at 0.13 mg/kg. | Li et al. (2016) | High |

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# 8 WEIGHT OF SCIENTIFIC EVIDENCE CONCLUSIONS FOR FATE AND TRANSPORT

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

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

- Has chromophores that absorb in the visible range of the solar light spectrum and is expected to undergo direct photolysis (Section 4.3).
- Will partition to organic carbon and particulate matter in air (Section 5.1).
- Will biodegrade in aerobic surface water, soil, and wastewater treatment processes (Sections 4.1, 5.3.2, 6.2).
- Does not biodegrade in anaerobic environments (Section 4.1).
- Will be removed after undergoing wastewater treatment and will sorb to sludge at high fractions, with a small fraction being present in effluent (Section 6.2).
- Is not bioaccumulative (Section 7).
- Is not expected to biodegrade under anoxic conditions and may have high persistence in anaerobic soils and sediments (Sections 4.1, 5.3.2, and 5.2.2).
- May have an apparent extended half-life in surface water and sediment proximal to continuous points of release.

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

- Is expected to be partially removed in conventional drinking water treatment systems via sorption to suspended organic matter and filtering media (Section 6.3).
- Has no significant degradation via hydrolysis under standard environmental conditions but hydrolysis rate was seen to increase with increasing pH and temperature in deep-landfill environments (Section 5.3.3).

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.

# 9 PHYSICAL CHEMISTRY AND FATE AND TRANSPORT ASSESSMENT CONCLUSIONS

The inherent physical and chemical properties of DIBP govern its environmental fate and transport. Based on DIBP's aqueous solubility and moderate tendency to adsorb to organic carbon, this chemical substance will be preferentially sorbed into sediments, soils, and suspended solids in wastewater treatment processes. Soil, sediment, and sludge/biosolids are predicted to be the major receiving compartments for DIBP as indicated by its physical and chemical and fate properties and fugacity assessment, and as supported by monitoring information. Surface water is predicted to be a minor pathway, and the main receiving compartment for phthalates discharged via wastewater treatment processes. However, phthalates in surface water will sorb strongly to suspended and benthic sediments. In areas where DIBP is continually released to water, higher levels of phthalates in surface water can be expected, trending downward distally from the point of releases. This also hold true for DIBP concentration in both suspended and benthic sediments. While DIBP undergoes relatively rapid aerobic biodegradation, it is persistent in anoxic/anaerobic environments (sediment, landfills) and like other phthalates it is expected to slowly hydrolyze under normal environmental conditions.

If released directly to the atmosphere, DIBP is expected to adsorb to particulate matter. It is not expected to undergo long-range transport facilitated by particulate matter due to the relatively rapid rates of both direct and indirect photolysis. Atmospheric concentrations of DIBP may be elevated proximal to sites of releases. Off gassing from landfills and volatilization from wastewater treatment processes are expected to be negligible releases in terms of ecological or human exposure in the environment due to its low vapor pressure. DIBP released to air may undergo rapid photodegradation and it is not expected to be a candidate chemical for long range transport.

In indoor settings, DIBP released to air is expected to preferentially accumulate in suspended particles and dust (Das et al., 2014; Kanazawa et al., 2010; Wormuth et al., 2006). The available information suggests that DIBP's indoor dust concentrations are associated with the presence of phthalate containing articles and the proximity to the facilities producing them (Das et al., 2014) as well as daily anthropogenic activities that might introduce DIBP containing products into indoor settings (Dodson et al., 2017).

DIBP has a predicted average environmental half-life of 14 days. In situations where aerobic conditions are predominant, DIBP is expected to degrade rapidly and be more persistent under anoxic/anaerobic conditions. In some sediments, landfills, and soils, DIBP may be persistent as it is resistant to anaerobic biodegradation. In anerobic environments, such as deep landfill zones, hydrolysis is expected the most prevalent process for the degradation of DIBP.

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