

#### Draft Chemistry, Fate, and Transport Assessment for Butyl Benzyl Phthalate (1,2-Benzenedicarboxylic acid, 1-butyl 2-(phenylmethyl) ester) (BBP)

**Technical Support Document for the Draft Risk Evaluation** 

**CASRN: 85-68-7** 



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# 98 ABBREVIATIONS AND ACRONYMS

90	ADDRL	ADDREVIATIONS AND ACRONTINS		
99	AS	Activated sludge		
100	BAF	Bioaccumulation factor		
101	BBP	Butyl Benzyl Phthalate		
102	BCF	Bioconcentration factor		
103	BMF	Biomagnification factor		
104	BOD	Biological oxygen demand		
105	BSAF	Biota-sediment accumulation factor		
106	CASRN	Chemical Abstracts Service Registry Number		
107	CDR	Chemical Data Reporting		
108	CFR	Code of Federal Regulations		
109	CTD	Characteristic travel distance		

110DBPDibutyl phthalate

111	DCHP	Dicyclohexyl phthalate
112	DEHP	Di-ethylhexyl phthalate
113	DEP	Diethyl phthalate
114	DIBP	Di-isobutyl phthalate
115	DINP	Di-isononyl phthalate
116	DMP	Dimethyl phthalate
117	DMR	Discharge Monitoring Reports
118	DMSO	Dimethylsulfoxide
119	DPE	Diphthalate ester
120	DRE	Destruction and removal efficiency
121	dw	Dry weight
122	EC50	Effect concentration at which 50 percent of test organisms exhibit an effect
123	ECHA	European Chemicals Agency
124	ECJRC	European Commission, Joint Research Centre
125	EPI	Estimation Programs Interface
126	FR	Federal register
127	HCl	Hydrochloric acid
128	HLC	Henry's Law constant
129	HOAc	Acetic acid
130	JNU	Jawaharlal Nehru University
131	Km	Maximum specific uptake rate (Monod kinetics)
132	LC50	Lethal concentration at which 50 percent of test organisms die
133	LOD	Limit of detection
134	Log K <sub>AW</sub>	Logarithmic air:water partition coefficient
135	Log K <sub>OA</sub>	Logarithmic octanol:air partition coefficient
136	Log K <sub>OC</sub>	Logarithmic organic carbon:water partition coefficient
137	Log Kow	Logarithmic octanol:water partition coefficient
138	Log K <sub>SW</sub>	Logarithmic soil:water partition coefficient
139	LOQ	Limit of quantification
140	LRTP	Long-range transport potential
141	MDL	Method detection limit
142	NaOAc	Sodium acetate
143	NaOH	Sodium hydroxide
144	ND	Non-detect/not detected
145	NITE	National Institute of Technology and Evaluation
146	OC	Organic carbon
147	OCSPP	Office of Chemical Safety and Pollution Prevention
148	OECD	Organisation for Economic Co-operation and Development
149	OPPT	Office of Pollution Prevention and Toxics
150	·OH	Hydroxyl radical
151	PAE	Phthalate acid ester
152	POTW	Publicly owned treatment works
153	PVB	Polyvinyl butyral
154	PVC	polyvinyl chloride
155	QSPR	Quantitative structure-property relationship
156	SCAS	semi-continuous activated sludge system
15/	SPM	Suspended particulate matter
150	SKU	Syracuse Research Corporation
159	$t_{1/2}$	нан-ше

160 TCLP Toxicity Characteristic Leaching Procedure Trophic magnification factor 161 TMF Total organic carbon 162 TOC Toxics Release Inventory 163 TRI Toxic Substances Control Act 164 TSCA Ultraviolet 165 UV 166 Wet weight WW WWTP Wastewater treatment plant 167

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- 186

#### 187 Disclaimer

- 188 Reference herein to any specific commercial products, process, or service by trade name, trademark,
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- 203 leadership.
- 204

### 205 SUMMARY

### **BBP** – Environmental Fate and Transport (Section 2.2):

This technical support document is in support of the TSCA *Draft Risk Evaluation for Butyl Benzyl Phthalate (BBP)* (U.S. EPA, 2025). EPA gathered and evaluated physical and chemical property information as well as fate and transport information according to the process described in the *Draft Risk Evaluation for Butyl Benzyl Phthalate (BBP) – Systematic Review Protocol* (U.S. EPA, 2024e). During the evaluation of butyl benzyl phthalate (BBP), EPA considered both measured and estimated data and information. Selected physical and chemical data are summarized in Table 2-1. Information on the full, extracted physical and chemical property data set is available in the file *Draft Risk Evaluation for Butyl Benzyl Phthalate (BBP) – Systematic Review Supplemental File: Data Quality Evaluation and Data Extraction Information for Physical and Chemical Properties* (U.S. EPA, 2024b). The fate and transport data collected are presented throughout Sections 3 through 8 with accompanying analyses. Information on the full, extracted fate and transport data set is available in the file *Draft Data Quality Evaluation and Data Extraction Information for Environmental Fate and Transport for Butyl Benzyl Phthalate (BBP)* (U.S. EPA, 2024a). The key points of this document are provided below.

### **BBP** – Physical Chemistry: Key Points

- Under standard environmental conditions, BBP is a clear, oily liquid with a melting point around -35 °C (NLM, 2015).
- BBP has a water solubility of 2.69 mg/L at 25 °C (NLM, 2015; Howard et al., 1985) and a log K<sub>OW</sub> of 4.73 (NLM, 2015).
- With a vapor pressure of 8.25×10<sup>-6</sup> mmHg at 25 °C (<u>NLM, 2015</u>; <u>Howard et al., 1985</u>) and a boiling point of 370 °C (<u>NLM, 2015</u>; <u>Haynes, 2014a</u>), BBP will exist in both vapor phase and sorbed to particulates in the atmosphere.
- The selected Henry's Law constant for BBP is 7.61×10<sup>-7</sup> atm·m<sup>3</sup>/mol at 25 °C (Elsevier, 2019), indicating that volatilization from water is not expected to be a dominant process for BBP.

### **BBP** – Environmental Fate and Transport: Key Points

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

- will partition to organic carbon and particulate matter in air, with a measured vapor pressure of  $8.25 \times 10^{-6}$  mmHg and a log K<sub>OA</sub> of 9.2 (Sections 5 and 6.1);
- is likely to be found in indoor air and dust (Section 6);
- will readily biodegrade in aerobic, aqueous environments including during wastewater treatment (Section 7.2) and surface waters (Section 4.1). Biodegradation rates of BBP in water will depend on the microbial community, organic matter presence, and previous exposure/adaptation to BBP.
- BBP will readily biodegrade in aerobic surface sediments (Section 4.1), however fractions bound to sediment are expected to present longer persistence until release by a shift in equilibrium;
- is expected to biodegrade under anaerobic conditions, generally more slowly than under aerobic conditions. As with aerobic degradation, anaerobic biodegradation rates of BBP are likely to depend on the microbial community, organic matter presence, and previous exposure/adaptation to BBP (Sections 4.1 and 6.2.2).

- BBP will be removed in wastewater treatment plants at 40 to 90 percent, with sorption to sludge and biodegradation both being significant removal mechanisms (Section 7.2);
- presents low bioconcentration potential in fish; however, monophthalates (monobutyl and monobenzyl phthalate) exhibited slightly elevated bioconcentration potential as compared to parent BBP (Section 8);
- will not biomagnify and will exhibit trophic dilution in aquatic species (Section 8);
- is likely to be present in biosolids, though is unlikely to be persistent or mobile in soils after land application of biosolids given its K<sub>OC</sub>, water solubility, and biodegradation processes; and
- will not exhibit substantial mobility to groundwater from soil or landfill environments and will tend to stay sorbed to solid organics in soil media and landfills.

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

- will not persist in air, and will undergo indirect photodegradation by reacting with hydroxyl radicals in the atmosphere with a half-life of 1.13 to 1.15 days (Section 4.3);
- will be removed in conventional drinking water treatment systems (Section 7.3);
- may show persistence in surface water, sediment, and soil proximal to continuous points of release, in cases where the release rate exceeds the rate of biodegradation (Sections 3.2, 5);
- does not biodegrade in anaerobic environments (Section 5.2, 5.3);
- will undergo aerobic and anaerobic biodegradation in soil and landfill media under conducive conditions (Sections 6.3.1 and 6.3.3, respectively);
- is expected to have a low tendency to migrate to groundwater, however explicit groundwater fate studies are limited for BBP; and
- will not undergo appreciable hydrolysis in aqueous systems, as biodegradation is expected to occur much more rapidly under most conditions (Sections 4.1 and 4.2); however, hydrolysis may be important in deep, acidic, thermophilic landfill environments (Section 6.3.3).

As a result of no empirical studies identified, there is a slight confidence that BBP:

208

# 209 1 INTRODUCTION

- Benzyl butyl phthalate (BBP) is a medium-chain, ester phthalate that is used in several processing and
- 211 industrial applications. Phthalate distribution in the environment is primarily due to anthropogenic
- activities. BBP may be found in the natural environment due to releases from activities related to
   industrial uses, and also through the widespread use in industrial and commercial materials, for instance
- as a filler or plasticizer in construction materials and automotive parts.
- 215

BBP exists as a clear, oily liquid at ambient temperature and pressure (NLM, 2015) with a melting point 216 of -35 °C, and a boiling point of 370 °C (NLM, 2015). With a vapor pressure of 8.25×10<sup>-6</sup> mmHg at 25 217 °C (NLM, 2015; Howard et al., 1985) and a Henry's Law constant of 7.61×10<sup>-7</sup> atm·m<sup>3</sup>/mol at 25 °C 218 (Elsevier, 2019), BBP is expected to have slight volatility from water, and be present in both free and 219 220 sorbed phase in the atmosphere. Though BBP has been shown to be readily biodegradable under several 221 relevant environmental conditions in water, soil, and sediment media (Section 4.1), its tendency to sorb 222 strongly to organic phases may contribute to some persistence, especially in areas receiving constant 223 releases that may outpace the rate of biodegradation (see Section 5). Because BBP is used in a wide 224 range of applications, it may be found in various environmental media including air (Section 6.1), 225 surface water (Section 6.2.1), sediment (Section 6.2.2), soil (Section 6.3.1), and biota (Section 8).

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# 228 2 APPROACH AND METHODOLOGY FOR PHYSICAL AND 229 CHEMICAL PROPERTY ASSESSMENT

230 EPA gathered and evaluated physical and chemical property data and information according to the 231 process described in the Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances (U.S. EPA, 2021) (also referred to as the "2021 Draft Systematic Review 232 233 Protocol"). During the evaluation of BBP, EPA considered both measured and estimated physical and 234 chemical property data/information. However, EPA selected empirical and measured data over modeled 235 data as much as possible to improve the confidence in the endpoints. For some physical and chemical 236 properties, there are multiple high-confidence values available for selection that were identified. The 237 majority of the preliminarily selected data were collected under standard environmental conditions (i.e., 238 20–25 °C and 760 mmHg). For values of endpoints for which no empirical data were identified (*i.e.*, the 239 octanol/air partition coefficient, log K<sub>OA</sub>), estimations from EPI Suite<sup>TM</sup> version 4.11 are reported (U.S. EPA, 2017). The full output from EPI Suite<sup>TM</sup> modeling is provided in Appendix A. With one exception, 240 241 only studies with an overall quality data determination of "High" were selected for use in selecting the representative physical and chemical properties of BBP, as a high volume of data was available. The 242 243 endpoint for which EPA did not identify any data with an overall quality data determination of "High" is 244 autoflammability, discussed in Section 2.2.11.

245

# 2.1 Selected Physical and Chemical Property Values for BBP

246

### 247 Table 2-1. Selected Physical and Chemical Property Values for BBP

Property	Selected Value(s) <sup>a</sup>	<b>Reference</b> (s)	Data Quality Rating
Molecular formula	$C_{19}H_{20}O_4$		
Molecular weight	312.37 g/mol		
Physical form	Clear, Liquid Oil; Slight Odor	<u>NLM (2015)</u>	High
Melting point	−35 °C	NLM (2015)	High

Property	Selected Value(s) <sup>a</sup>	Reference(s)	Data Quality Rating		
Boiling point	370 °C	<u>NLM (2015)</u> citing ( <u>Haynes, 2014a</u> )	High		
Density	1.119 g/cm <sup>3</sup>	<u>NLM (2015)</u> citing ( <u>Haynes, 2014a</u> )	High		
Vapor pressure	8.25E–06 mmHg at 25 °C	<u>NLM (2015)</u> citing (Howard et al., 1985)	High		
Vapor density	10.8 (air = 1)	<u>NLM (2015)</u>	High		
Water solubility	2.69 mg/L at 25 °C	<u>NLM (2015)</u> citing <u>Howard</u> et al. (1985)	High		
Octanol:water partition coefficient (log K <sub>OW</sub> )	4.73	<u>NLM (2015)</u>	High		
Octanol:air partition coefficient (log K <sub>OA</sub> )	$9.2^{b}$	<u>U.S. EPA (2017)</u>	High		
Henry's Law constant (HLC)	7.61E–07 atm $\cdot$ m <sup>3</sup> /mol at 25 °C	Elsevier (2019)	High		
Flash point	199 °C	<u>NLM (2015)</u>	High		
Autoflammability	233 to 425 °C	<u>NTP (1997); ECJRC</u> (2008); ECJRC (2007); NCBI (2020)	Medium		
Viscosity	55 cP	Elsevier (2019)	High		
<sup><i>a</i></sup> Measured unless otherwise noted. <sup><i>b</i></sup> Information was estimated using EPI Suite <sup>™</sup> U.S. EPA (2017).					

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### 2.2 Endpoint Assessments

### 2.2.1 Melting Point

251 Melting point informs the chemical's physical state, environmental fate and transport, as well as the 252 chemical's potential bioavailability. The EPA extracted and evaluated nine melting point data for BBP, 253 five of which were evaluated to be high-quality. All five high-quality sources reported a BBP melting 254 point of -35 °C (Elsevier, 2019; DOE, 2016; NLM, 2015; ECHA, 2012; IARC, 1999). As is the case with most of the physical or chemical property endpoint data presented in this document, several of 255 256 these data sources were found to cross-reference various other sources, largely well-established chemical property reference texts (e.g., CRC Handbook of Chemistry and Physics (Haynes, 2014a), 257 258 Handbook of Environmental Data on Organic Chemicals (Verschueren, 1996)), and it is possible that the 259 reference texts provide the same value without providing information on the primary study. Therefore, some data may have been double counted in this set, as highlighted in Section 2.3. EPA selected a 260 261 melting point value of -35 °C (NLM, 2015) as a representative melting point for BBP, as it was reported 262 by all of the overall high-quality data sources. The identified value is consistent with the value proposed in the Final Scope for the Risk Evaluation of BBP (U.S. EPA, 2020). 263

### **264 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 18 data containing BBP boiling point information, seven of which were evaluated to be high-quality. The high-quality sources reported BBP boiling points ranging from 250 to 370 °C (Elsevier, 2019; U.S. EPA, 2019a; DOE, 2016; NLM,

269 2015; Haynes, 2014a; Park and Sheehan, 2000; IARC, 1999). The mean and mode of the high-quality reported boiling point values are 353 and 370 °C, respectively. EPA selected a boiling point value of 270 271 370 °C, as this value is the mode and was reported by six of the seven identified overall high-quality data sources (U.S. EPA, 2019a; DOE, 2016; NLM, 2015; Haynes, 2014a; Park and Sheehan, 2000; 272 273 IARC, 1999). As with other physical and chemical property endpoints, cross-referencing in several 274 secondary sources was observed and therefore, some data may have been double counted in this set, as 275 highlighted in Section 2.3. The identified value is consistent with the value proposed in the Final Scope 276 for the Risk Evaluation of BBP (U.S. EPA, 2020).

### 2.2.3 Density

The EPA extracted and evaluated 16 density data for BBP, seven of which were evaluated to be high-278 279 quality. The sources reporting overall high-quality data yielded BBP density values between 1.100 and 280 1.119 g/cm<sup>3</sup> (Elsevier, 2019; DOE, 2016; NLM, 2015; Havnes, 2014a; ECHA, 2012; Park and Sheehan, 281 2000; IARC, 1999). There is good agreement among the identified density values for BBP, with no 282 obvious outliers. The mean of the reported high-quality density values is 1.114 g/cm<sup>3</sup>. EPA selected a density of 1.119 g/cm<sup>3</sup> at 25 °C (NLM, 2015; Haynes, 2014a) to closely represent the mean of the 283 284 density values obtained from the available high-quality data sources. Additionally, the value of 1.119 285 g/cm<sup>3</sup> was reported twice within data pool of high-quality data sources and is consistent with the value 286 proposed in the Final Scope for the Risk Evaluation of BBP (U.S. EPA, 2020).

### 2.2.4 Vapor Pressure

Vapor pressure indicates the chemical's potential to volatilize, fugitive emissions and other releases to 288 289 the atmosphere, undergo long range transport, and undergo specific exposure pathways. The EPA extracted and evaluated 22 vapor pressure data for BBP. Eleven vapor pressure values from ten sources 290 291 were identified and evaluated as overall high-quality data. These data points were further filtered to only 292 include the nine vapor pressure values collected between 20 and 25 °C, of which the reported BBP vapor pressure values range from  $1.50 \times 10^{-6}$  to  $9.10 \times 10^{-5}$  mmHg (Elsevier, 2019; DOE, 2016; NLM, 2015; 293 Gobble et al., 2014; Howard et al., 1985). The mean vapor pressure of the deduplicated. reported 294 295 experimental values collected at 25 °C (i.e., reported in (Elsevier, 2019; DOE, 2016; Gobble et al., 2014; Howard et al., 1985)) is  $2.73 \times 10^{-5}$  mmHg. EPA selected the experimentally derived vapor pressure 296 value of 8.25×10<sup>-6</sup> mmHg at 25 °C (U.S. EPA, 2019a; DOE, 2016; NLM, 2015), as this was the mode 297 298 of the overall high-quality data collected between 20 and 25 °C (three of the nine values). The identified 299 value is consistent with the value proposed in the Final Scope for the Risk Evaluation of BBP (U.S. 300 EPA, 2020).

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### 2.2.5 Vapor Density

The EPA identified three vapor density data for BBP, two of which were rated as overall high-quality (NLM, 2015; IARC, 1999). EPA selected a vapor density value of 10.8 (air = 1) because it was reported by both data sources with high-quality data. The identified value is consistent with the value proposed in the *Final Scope for the Risk Evaluation of BBP* (U.S. EPA, 2020).

306 2.2.6 Water Solubility

Water solubility informs many endpoints not only within the realm of fate and transport of BBP in the
environment, but also when modelling for industrial process, engineering, human and ecological hazard,
and exposure assessments. The EPA extracted and evaluated 24 water solubility data for BBP. Fourteen
data points from twelve sources were evaluated as overall high-quality data. These sources reported
water solubility values from 0.67 to 2.8 mg/L (Elsevier, 2019; U.S. EPA, 2019a; EC/HC, 2017; NLM,
2015; ECHA, 2012; EC/HC, 2000; Mueller and Klein, 1992; Analytical Bio-Chemistry Labs, 1986;
Howard et al., 1985; Boese, 1984; SRC, 1983b; Hollifield, 1979). These data sources employed different

- 314 analytical methods and experimental temperatures that may have contributed to the variance of
- 315 identified water solubilities; the mean water solubility value of BBP at relevant environmental
- 316 temperatures (20 to 25 °C) is 2.26 mg/L (Elsevier, 2019; NLM, 2015; ECHA, 2012; EC/HC, 2000;
- Analytical Bio-Chemistry Labs, 1986; Howard et al., 1985; SRC, 1983b; Hollifield, 1979). A water 317
- solubility of 2.69 mg/L was selected as the environmentally relevant water solubility of BBP, as it was 318
- 319 reported by several sources (U.S. EPA, 2019b; EC/HC, 2017; NLM, 2015; Mueller and Klein, 1992;
- 320 Howard et al., 1985; SRC, 1983b). The identified value is consistent with the value proposed in the
- Final Scope for the Risk Evaluation of BBP (U.S. EPA, 2020). 321

### 2.2.7 Octanol: Water Partition Coefficient (log K<sub>OW</sub>)

322 The octanol:water partition coefficient (log  $K_{OW}$ ) quantifies how a chemical will partition between 323 324 octanol (a common surrogate for biological lipids and other hydrophobic media) and water. In the 325 absence of adequate empirical data, log K<sub>OW</sub> is often used to predict a chemical's tendency to partition 326 to biota (*i.e.*, bioconcentration), as well as for the estimation of other properties including water 327 solubility, soil adsorption, and bioavailability. The EPA extracted and evaluated 18 data sources containing BBP Kow information. Eleven Kow values from ten sources were evaluated as overall high-328 329 quality. These sources reported BBP log K<sub>OW</sub> values ranging from 3.57 to 4.91, with a mean of 4.70 (Elsevier, 2019; Ishak et al., 2019; U.S. EPA, 2019a; EC/HC, 2017; NLM, 2015; ECHA, 2012; EC/HC, 330 2000; IARC, 1999; Mueller and Klein, 1992; Howard et al., 1985). EPA selected an experimental log 331 332 K<sub>OW</sub> value of 4.73 (NLM, 2015) for use in this risk evaluation as it lies very close to the mean of the 333 overall high-quality data identified. The identified value is consistent with the value proposed in the 334 Final Scope for the Risk Evaluation of BBP (U.S. EPA, 2020).

335

343

### 2.2.8 Octanol: Air Partition Coefficient (log K<sub>OA</sub>)

No data were identified reporting empirical octanol:air (log K<sub>OA</sub>) values for BBP. EPA leveraged the 336 KOAWIN<sup>TM</sup> model as part of EPI Suite<sup>TM</sup> to obtain an estimated log K<sub>OA</sub> value of 9.27 (U.S. EPA, 337 2017). One modeled value was identified during systematic review and was rated as a medium-quality: 338 using a quantitative structure-property relationship (QSPR) model, Lu (2009) estimated a log K<sub>OA</sub> value 339 of 8.98, in good agreement with the value of 9.27 modeled using KOAWIN<sup>TM</sup>. For the purposes of this 340 risk evaluation, EPA selected the EPI Suite<sup>™</sup> log K<sub>OA</sub> value of 9.27. See Section 5.1 for additional 341 information on the partitioning coefficients for BBP. 342

2.2.9 Henry's Law Constant

The Henry's Law constant (HLC) provides an indication of a chemical's volatility from water and gives 344 345 an indication of environmental partitioning, potential removal during wastewater treatment via aeration 346 stripping, and possible routes of environmental exposure. The EPA extracted and evaluated seven HLC values for BBP. Three of the sources were identified and evaluated as overall high-quality data sources. 347 of which the HLC range is  $7.61 \times 10^{-7}$  to  $2.02 \times 10^{-6}$  atm·m<sup>3</sup>/mol, with a mean of  $1.36 \times 10^{-6}$  atm·m<sup>3</sup>/mol 348 349 (Elsevier, 2019; Cousins and Mackay, 2000; EC/HC, 2000). One overall high-quality data source reported a BBP HLC value calculated using QSAR methodology (Cousins and Mackay, 2000), while a 350 second study did not specify the derivation method (EC/HC, 2000). EPA selected the experimental HLC 351 value of  $7.61 \times 10^{-7}$  atm m<sup>3</sup>/mol at 25 °C for use in this risk evaluation, as it is the only identified high-352 353 quality value obtained empirically (Elsevier, 2019). The identified value is consistent with the value 354 proposed in the Final Scope for the Risk Evaluation of BBP (U.S. EPA, 2020).

#### 355 2.2.10 Flash Point

The EPA extracted and evaluated four data sources containing seven BBP flash point temperatures, one 356 357 data point of which was evaluated as overall high-quality. EPA selected the high-quality flash point 358 value of 199 °C (NLM, 2015) for use in this draft risk evaluation. This high-quality, selected value

replaces the medium-quality, proposed flash point range of 110 to 113 °C retrieved from ChemSpider (<u>RSC, 2019</u>) highlighted in the *Final Scope for the Risk Evaluation of BBP* (<u>U.S. EPA, 2020</u>). In addition to the improved data-quality rating of the newly selected flash point value, the flash point temperature range suggested in the scope are no longer available in ChemSpider and therefore there is

363 low confidence in their validity.

### 364 2.2.11 Autoflammability

365 A value for the autoflammability of BBP was not identified in the initial data review for the Final Scope 366 for the Risk Evaluation of BBP (U.S. EPA, 2020). The systematic review process conducted since 367 identified four overall medium-quality data sources reporting five autoflammability values ranging from 233 to 425 °C (NCBI, 2020; ECJRC, 2008, 2007; NTP, 1997). Because the data reporting in the 368 identified studies were lacking critical detail on experimental and analytical methodologies, EPA 369 370 moderate confidence in the exact autoflammability values. However, considering the range of 371 autoflammability values identified, EPA has high confidence that BBP is not expected to autoignite under normal environmental conditions. 372

### **2.2.12 Viscosity**

The EPA extracted and evaluated one data source containing BBP viscosity information that was evaluated as an overall high-quality data source (Elsevier, 2019). EPA selected the value reported by Elsevier (2019) of 55 cP at 20 °C for BBP's viscosity for this draft risk evaluation. The identified value is consistent with the value proposed in the *Final Scope for the Risk Evaluation of BBP* (U.S. EPA, 2020).

# 379 380 2.3 Strengths, Limitations, Assumptions, and Key Sources of Uncertainty for the Physical and Chemical Property Assessment

The physical and chemical property data presented in this document were the product of a systematic review of reasonably available information. The data analyses, therefore, consider only a subset of all existing physical and chemical data, not an exhaustive acquisition of all potential data. The representative physical and chemical property values were selected based on professional judgement and the overall data quality ranking of the associated references. Where systematic review did not identify any data sources for a given physical or chemical property, Estimation Programs Interface (EPI) Suite<sup>™</sup> (U.S. EPA, 2017) was leveraged to provide a model estimate of the parameter.

389 Due to cross-referencing between many of the databases identified and assessed through the systematic 390 review process, there is potential for data from one primary source to be collected multiple times 391 resulting in duplication within the data set. This duplication should be considered as a potential source 392 of uncertainty in the data analyses. Nonetheless, the number of data sources identified for a given 393 property contributes to the relative confidence in a selected value: when numerous data sources are 394 collected and considered in the selection of a property value (*e.g.*,  $\log K_{OW}$  values for BBP), there is 395 more robust confidence in that selected value as compared to a selected value from a property with one 396 or few data sources (e.g., viscosity of BBP). Confidence in a selected value is especially robust when 397 numerous independent sources agree on a small range of values for a given property.

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#### **APPROACH AND METHODOLOGY FOR FATE AND** 399 3 **TRANSPORT ASSESSMENT** 400

#### 3.1 Collection, Screening, and Integration of Fate and Transport Data for 401 **BBP** 402

403 Reasonably available environmental fate data—including biotic and abiotic biodegradation rates, 404 removal during wastewater treatment, volatilization from lakes and rivers, and organic carbon:water 405 partition coefficient (log K<sub>OC</sub>)—are the parameters used in the current draft risk evaluation. In assessing 406 the environmental fate and transport of BBP, EPA considered the full range of results from extracted 407 data that were rated high-quality. For endpoints for which few or no high-quality studies were identified 408 during systematic review (e.g., indirect photolysis in air, biodegradation in soil), medium-rated studies 409 were also considered. Information on the full extracted data set is available in the file *Draft Data Quality* 410 Evaluation and Data Extraction Information for Environmental Fate and Transport for Butyl Benzyl 411 *Phthalate (BBP)* (U.S. EPA, 2024a). Endpoints for which few or no empirical data were identified 412 during systematic review were estimated using the models comprising EPI Suite<sup>™</sup> (U.S. EPA, 2017), a predictive tool for physical and chemical properties and environmental fate estimation. The full output 413 from EPI Suite<sup>TM</sup> modeling is provided in Appendix A. 414

415

416 A brief description of evidence integration for fate and transport is available in the *Draft Systematic* 

417 Review Protocol for Butyl Benzyl Phthalate (U.S. EPA, 2024e). Table 3-1 provides a summary of the

418 selected data that EPA considered while assessing the environmental fate of BBP and were updated after

419 publication of Final Scope of the Risk Evaluation for Butyl Benzyl Phthalate (BBP) CASRN 84-69-5

420 (U.S. EPA, 2020) with additional information identified through the systematic review process. Sections

- 421 4 and 5 summarize the findings and provide the rationale for selecting these environmental fate 422 characteristics.
- 423

Property or Endpoint	Value(s)	Reference	Data Quality Rating
Direct Photolysis (air)	Contains chromophores that absorb light at greater than 290 nm wavelength	<u>NCBI (2020)</u>	NA
Direct Photolysis (water)	1%/28 days; aqueous solutions of test material were exposed to ca. 251 hours of sunshine in tightly sealed quartz test tubes.	Monsanto (1983f)	High
Indirect Photolysis	$t_{1/2} = 23.3$ hours (based on •OH reaction rate constant of $1.10E-11$ cm <sup>3</sup> /mol·sec and $1.5E06 \cdot OH/cm^{3})^{a}$	<u>U.S. EPA (2017)</u>	High
(air)	$t_{1/2} = 18$ hours (based on •OH reaction rate constant of 1.1049E–11 cm <sup>3</sup> /mol·sec and 1.5E06 ·OH/cm <sup>3</sup> ; calculation)	Peterson and Staples (2003)	Medium
Hydrolysis	t <sub>1/2</sub> at pH 7: 1.4 years at 25 °C (estimated) <sup><i>a</i></sup> t <sub>1/2</sub> at pH 8: 51 days at 25 °C (estimated) <sup><i>a</i></sup>	<u>U.S. EPA (2017)</u>	High
Biodegradation	Readily biodegradable	See Table 4-1 for comple on considered biodegra	ete information dation studies
Wastewater Treatment	Expected removal between 40 and 90%	See Table 7-1 for complete informatic on considered WWTP studies	
Bioconcentration Factor	Low bioconcentration potential		

424 **Table 3-1. Environmental Fate and Transport Properties of BBP** 

Property or Endpoint	Value(s)	Reference	Data Quality Rating			
Bioaccumulation Factor	Low bioconcentration potential	See Table 8-1 for comple	ete information			
Biota Sediment Accumulation Factor	Some sediment bioaccumulation potential	on considered bioconcentration bioaccumulation studies				
Trophic Magnification Factor	Trophic dilution					
Organic Carbon:Water Partition Coefficient (Log K <sub>OC</sub> )	Mean soil/sediment log $K_{OC} = 4.86 \text{ L/kg}$ (n = 4 studies)	See for Table 5-1 comple on considered log K	ete information foc studies			
<sup>a</sup> Values were estimated using	Values were estimated using EPI Suite <sup>TM</sup> U.S. EPA (2017).					

425

426 EPA also analyzed transformation processes of BBP, as presented in Section 4. Understanding the 427 transformation behavior of BBP informs which pathways are expected to be dominant or contributing to 428 persistence in different compartments. Transformation half-lives were collected and compared between 429 and within transformation mechanism types (*i.e.*, photolysis, biodegradation, hydrolysis). For BBP, 430 biodegradation is expected to be the dominant transformation process in all media except for air. In 431 instances where biodegradation half-lives were not available from the identified sources (as noted in 432 Table 4-1), a first-order approximation of the biodegradation half-life was calculated from the fraction 433 of BBP remaining and the study duration, using the first-order rate equation:

### 435 Equation 3-1

Where:

436

434

 $t_{1/2} = \frac{\ln\left(2\right)}{-\ln\left(f_{BBP\_remain}\right)/t}$ 

437 438

439

440

441

 $t_{1/2}$  = half-life (hours)  $f_{BBP\_remain}$  = fraction of BBP remaining at time t t = study duration (hours)

442 443 This first-order approximation was conducted to directly compare studies across the same units (i.e., 444 half-life). Note that half-lives derived using Equation 3-1 are estimates calculated from a single 445 timepoint rather than a full kinetic study. While this strategy provides an estimate of BBP's 446 biodegradation kinetics, there is greater uncertainty in these calculated half-lives as compared to those 447 directly observed or derived from a full kinetic biodegradation data set. Regardless, the half-lives 448 derived using Equation 3-1 are based on data from data evaluated as overall high-quality and are in 449 relative agreement with those directly extracted from a data source and/or derived with a full kinetic 450 dataset. Therefore, the overall conclusions (see Section 10) about the biodegradability of BBP are 451 unaffected by this exercise.

# 452 **3.2 Tier I Analysis Methods**

EPA conducted a Tier I assessment to identify the environmental compartments (*i.e.*, water, sediment,
biosolids, soil, groundwater, air) of major and minor relevance to the fate and transport of BBP as
indicated by its partitioning behavior. Selected values for BBP's log K<sub>OW</sub>, log K<sub>OC</sub>, log K<sub>OA</sub>, and log
K<sub>AW</sub> were used to identify in which media BBP is most likely to be located as estimated by BBP's
equilibrium partitioning behavior among surface water, soil, sediment, and air media. See Section 5.1
for explanation of the selected partition coefficients. Results of the Tier I analysis are provided in
Section 5.2.

#### 3.3 Tier II Analysis Methods, and EPI Suite<sup>TM</sup> Model Inputs and Settings 460 While Tier I analyses describe BBP's behavior under equilibrium conditions, Tier II analysis 461 462 incorporates transformation estimates of BBP in the environment (from Section 4), as well as employs a 463 steady-state model to emulate various emission scenarios. The approach described by Mackay et al. (1996) using the Level III Fugacity model in EPI Suite<sup>™</sup> (LEV3EPI<sup>™</sup>) was used for this Tier II analysis. 464 465 LEV3EPI<sup>TM</sup> is described as a steady-state, non-equilibrium model that uses a chemical's physical and 466 chemical properties and transformation rates to predict partitioning of the chemical between environmental compartments and its persistence in a model environment (U.S. EPA, 2017). A Tier II 467 468 analysis involves reviewing environmental release information for BBP to determine whether further assessment is warranted for each environmental medium. 469 470

471 Current environmental release data for BBP were not available from the Toxics Release Inventory 472 (TRI); however, between 1,000,000 and less than 20,000,000 pounds of CASRN 85-68-7 were produced 473 annually from 2016 to 2019 for use in commercial products, chemical substances or mixtures sold to 474 consumers, or at industrial sites according to production data from the Chemical Data Reporting (CDR) 475 2020 reporting period. The production volume for BBP in 2015 was between 10 and 50 million pounds 476 and decreased to between one million and less than 20 million pounds in 2019 based on the 2020 CDR 477 data {U.S. EPA, 2020, 6275311}. Environmental release data from the Discharge Monitoring Reports 478 (DMRs) were available for BBP from 2021 to 2023. The total annual releases from watershed discharge 479 were 101, 2,897, and 245 pounds in 2021, 2022, and 2023, respectively.

480

481 BBP is used as a plastic in polyvinyl chloride (PVC) flooring and other materials, in paints and coatings, in adhesive formulations and in printing inks (EC/HC, 2000). BBP is not chemically bound to the 482 polymer matrix and can migrate from the surface of polymer products (ECJRC, 2007). Therefore, BBP 483 484 can easily be released to the environment from polymer-based products during their use, and disposal. 485 Additionally, BBP 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 486 487 results in effluent discharge to water and land application of biosolids, which would lead to media 488 specific evaluations. Releases from landfills and incinerators will occur from the disposal of liquid and 489 solid wastes and warrants media specific evaluations. 490

- The above-discussed environmental release information is also useful for fugacity modeling because the
  emission rates will predict a real-time percent mass distribution for each environmental medium.
  However, limited complete emission data was identified for use in BBP fugacity modeling. Therefore, to
  assess a range of possible emission distributions, EPA modeled four emission scenarios: equal releases
  to water, air, and soil; water releases only; air releases only; and soil releases only.
- 496

As biodegradation is expected to be the dominant transformation pathway for BBP (see Section 4), the persistence half-lives used in the LEV3EPI™ fugacity model were based on the biodegradation of BBP rather than other transformation pathways. While empirical biodegradation data are available, biodegradation half-lives modeled under standard environmental conditions were also considered: empirical biodegradation half-lives collected employing natural inoculums may only be applicable to locations with the same set of environmental conditions. Modeled values can provide half-life estimates based on a set of standard conditions allowing rates between media types to be more readily compared.

504
505 BBP's readily biodegradable designation was used to model environmental half-lives in all media for
506 use in the LEV3EPI<sup>™</sup> fugacity model: half-lives indicative of readily biodegradable substances of 5
507 days (120 hours) in water, 10 days (240 hours) in soil, and 45 days (1,080 hours) in sediment were
508 selected for this fugacity model (U.S. EPA, 2017). Compared to the empirical biodegradation evidence

- 509 presented in Section 4.1, the estimated values represent the conservative (*i.e.*, more persistent) end of the 510 range of identified primary biodegradation half-life values (Section 4.1) from high- and medium-quality 511 studies. The use of this more conservative approach is reasonable with the understanding that fugacity 512 modeling provides an estimate of BBP's partitioning in the environment rather than exact media concentration numbers. The use of the estimated half-lives did not change conclusions on which 513 environmental pathways will be important for BBP. A half-life of 0.97 days was selected for the air 514 compartment as it was the most conservative estimate for BBP persistence with respect to indirect 515 516 photolysis (see Section 4.3) (U.S. EPA, 2017). The LEV3EPI™ results were consistent with environmental monitoring data. Further discussion of BBP partitioning can be found in Section 5. 517
- 518
- 519 The following additional inputs parameters were used for the Level III Fugacity model in EPI Suite<sup>TM</sup>:
  - Melting Point = -35.00 °C (see Section 2.2.1 and Table 2-1)
  - Boiling Point = 370 °C (see Section 2.2.2 and Table 2-1)
  - Vapor Pressure =  $8.25 \times 10^{-6}$  mm Hg (see Section 2.2.4 and Table 2-1)
  - Water Solubility = 2.69 mg/L (see Section 2.2.6 and Table 2-1)
  - Log  $K_{OW} = 4.73$  (see Section 2.2.7 and Table 2-1)
  - Log  $K_{OC} = 4.86$  L/kg (see Section 5, Table 5-1, and Table 5-2)
  - HLC =  $7.61 \times 10^{-7}$  atm·m<sup>3</sup>/mol (see Section 2.2.9 and Table 2-1)
  - SMILES: O=C(OCc(cccc1)c1)c(c(ccc2)C(=O)OCCCC)c2
- 527 528 529

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# 530 **4 TRANSFORMATION PROCESSES**

BBP released to the environment will transform to the monoesters (monobutyl and monobenzyl 531 phthalate) via abiotic processes such as photolysis (direct and indirect) and hydrolysis of the carboxylic 532 acid ester group (U.S. EPA, 2023). Biodegradation pathways for the phthalates consist of primary 533 biodegradation from phthalate diesters to phthalate monoesters, then to phthalic acid, and ultimately 534 535 biodegradation of phthalic acid to form CO<sub>2</sub> and/or CH<sub>4</sub> (Huang et al., 2013; Wolfe et al., 1980). Both 536 monobutyl phthalate and monobenzyl phthalate are both more soluble and more bioavailable than BBP. 537 The monoesters are also expected to undergo biodegradation more rapidly than the diester form. EPA 538 considered BBP transformation products and degradants qualitatively. However, due to their lack of 539 persistence, the products and degradants are not expected to contribute appreciably to risk, thus EPA is 540 not considering them further in this RE. Both biotic and abiotic routes of degradation for BBP are 541 described in the following sections.

### 542 **4.1 Biodegradation**

BBP is considered readily biodegradable in most aquatic and terrestrial environments. As mentioned 543 544 above, BBP typically undergoes enzymatic hydrolysis of the carboxylic acid ester groups during 545 biodegradation to form monobutyl and monobenzyl phthalates as primary degradation products. It is 546 important to note that the biodegradation potential of BBP in the environment is not only inherent to 547 BBP's structure, biodegradation rates are also influenced by temperature, oxygen availability, presence 548 of co- or intermediate substrates, organic carbon concentration, and concentration of the chemical of 549 interest. Such environmental conditions also influence the composition of microbial communities, and 550 therefore the biodegradation rate and pathway in that environment.

- 551
- EPA extracted and evaluated 59 data points for biodegradation in water, 19 data points for
- 553 biodegradation in sediment, and two data points for biodegradation in soil during systematic review.
- 554 However, for the purposes of the following biodegradation analysis, EPA considered studies that were

given an overall high-quality ranking. In cases of limited or no high-quality studies (*e.g.*, soil

biodegradation), medium-quality studies were also considered. The studies summarized in the following
 subsections are also presented in Table 4-1.

558

### 559 Aerobic Biodegradation in Water

Both screening studies and simulation/microcosm studies were considered in the assessment of aerobic
biodegradation of BBP. Screening studies typically employ media or inoculums that contain high
concentrations of competent (*i.e.*, able to degrade BBP) microbes and may result in faster
biodegradation rates as compared to studies employing natural media. Microcosm studies are typically
designed to simulate natural environmental conditions and may provide more accurate information on
how a chemical will behave in the environment as compared to screening tests. Regardless, variability in
biodegradation rates is inherent to the microbial community.

567

568 Studies conducted in sludge media or employing sludge or activated sludge (AS) inoculums indicate that 569 BBP can be considered as readily biodegradable. Desai et al. (1990) reported a maximum specific uptake rate (Km, based on Monod kinetics) of 12.8 day<sup>-1</sup> for BBP degradation in flasks containing 570 571 synthetic medium and microbial inoculum from a municipal wastewater treatment plant, measured via 572 O<sub>2</sub> consumption. In similar systems analyzed for oxygen consumption using biological oxygen demand 573 (BOD) analysis, Fujita et al. (2005) reported half-lives ranging from 3 to 7 days (unspecified whether 574 primary or ultimate), and primary biodegradation half-lives ranging from 2 to 3 days based on parent 575 compound loss. In a static BOD test system containing yeast and a settled domestic wastewater inoculum, Tabak et al. (1981) reported 100 percent primary degradation of both 5 and 10 mg/L of BBP 576 577 over 7 days. In a 24-hour, semi-continuous activated sludge system (SCAS), Saeger and Tucker (1976) 578 measured 93±6 percent degradation of parent BBP when dosed with 5 mg-BBP per cycle, and greater 579 than 99 percent degradation when dosed with 200 mg-BBP per cycle. Identified products in the SCAS

- system, monobutyl phthalate and phthalic acid, were also reported to be rapidly degraded. The same
   study measured CO<sub>2</sub> evolution of 95.86 percent of theoretical yield in BOD dilution water with a pooled
   activated sludge inoculum (Saeger and Tucker, 1976). Several of these studies, however, used nominal
   test BBP concentrations above its reported solubility, as discussed below.
- 584

585 Biodegradation studies employing natural media also indicate that BBP will biodegrade rapidly in aqueous environments. Adams et al. (1988) studied the biodegradation of <sup>14</sup>C-BBP in freshwater 586 587 microcosms operated under semi-steady state containing sediment and water from the Illinois River. The 588 authors found the parent BBP concentration was degraded to 50 percent of starting concentrations (10 589 and 100  $\mu$ g/L) by day 3 of the study, and to between 1 and 20 percent of starting concentration by day 5. 590 As reported in the study, kinetic data was used to calculate first-order aqueous primary degradation half-591 lives of 1.5 days in the 10  $\mu$ g/L microcosms, and 2.2 days in the 100  $\mu$ g/L microcosms. Ultimate 592 biodegradation observed from  ${}^{14}CO_2$  evolution was 10.8±1.8 percent over the 30-day experiment. Note 593 that Adams et al. (1988) and Monsanto (1986a) present the same experiment and are therefore replicates 594 of one another. A similar study reported a primary biodegradation half-life of 1.1 to 1.4 days, and an ultimate biodegradation half-life of 4.7 days for <sup>14</sup>C-BBP in a lake sediment and water microcosm with 595 596 media from Lake 34 in the Busch Wildlife Area (St. Charles County, MO) (Monsanto, 1983c). In a river 597 die-away study employing Mississippi River water, half-lives of 0.5 and 1.4 days were observed at BBP 598 test concentrations of 50.3 and 503 µg/L, respectively (Monsanto, 1983d). 599

Fujita et al. (2005) reported slightly longer half-lives for both the primary and ultimate biodegradation of
 BBP in synthetic river water inoculated with microbes collected from natural surface waters: primary
 biodegradation half-life ranges of 4 to 6 days and 5 to 6 days were observed with river microbe and

pond microbe inoculums, respectively (from Figure 1). One hundred percent loss of parent BBP was
 attained at 14 days for all inoculums (Fujita et al., 2005).

605

It is expected that both the composition of microbial communities as well as their exposure to PAEs in
 the environment will influence the observed biodegradation rates of BBP. This was demonstrated by
 <u>SRC (1983a)</u> when comparing two different inoculum acclimation procedures in shake flask
 biodegradation screening tests: when using an inoculum derived from mixed liquor, soil, and raw

- biodegradation screening tests: when using an inoculum derived from mixed liquor, soil, and raw
  wastewater influent and let to acclimate to a mixture of 14 PAEs, degradation rates of 42.5 and 77.7
- 611 percent over 28 days were observed for ultimate and primary biodegradation of BBP, respectively.
- However, when the inoculum was left to acclimate to BBP only, the BBP biodegradation rates increased
- to 87.5 and 97.2 percent over 28 days for ultimate and primary biodegradation, respectively (<u>SRC</u>,
- 614 <u>1983a</u>). This suggests a certain level of enzymatic specificity required to accommodate the benzyl
- moiety of BBP, therefore microbes adapted to other PAEs may not be as well-adapted to BBP.
- 616
- 617 Several studies employing both natural media/inoculums and activated sludge/wastewater inoculums
- 618 used nominal BBP test concentrations above BBP's selected water solubility of 2.69 mg/L (Howard et
- 619 al., 1985). The concentration levels of these studies are: 5 and 10 mg/L (Tabak et al., 1981); 20 mg/L (Shelton et al., 1984; Monsanto, 1983e; SRC, 1983a; Michigan State University, 1981; Saeger and 620 Tucker, 1976); 10 and 40 mg-TOC/L (Fujita et al., 2005); and 100 mg/L (Desai et al., 1990). In such 621 622 instances, BBP distribution in the aqueous system may be heterogeneous and may associate with dissolved and/or particulate matter in the test systems that are typically absent in water solubility tests, 623 artificially inflating the apparent aqueous BBP concentration. Because of this, the apparent 624 625 biodegradation may be an underestimation of the actual biodegradation rate, as BBP that may be 626 associated to dissolved and particulate organic matter is typically considered to be unavailable for 627 microbial biodegradation. This is also true in sediment environments, as discussed in the following 628 subsection. Additionally, at concentrations above the limit of water solubility, test compound 629 homogeneity may not be achieved, therefore biodegradation may become limited by dispersion 630 processes. This was investigated by Monsanto (1983e) who found the BBP biodegradation rate in a 631 shake-flask test to increase when 20 mg-BBP/L was tested with dispersion aids of both DMSO as well 632 as florisil mesh.
- 633

While the biodegradation rate of BBP in water will depend on the microbial community, organic matter presence, and adaptation to BBP, the evidence suggests that the biodegradation rate of BBP in water will be on the order of days to weeks.

637

# 638 Biodegradation in Sediment

Biodegradation in sediments may occur aerobically and anaerobically. Top layers of the sediment

- 640 compartment can have enough dissolved oxygen to support aerobic and/or facultative microbial
- 641 processes, especially in surface waters that experience appreciable exchange with the atmosphere as well
- 642 as mixing within the water column down to the sediment layer. As oxygen is consumed in the top layers 643 of sediment, the deeper sediments tend to harbor anaerobic conditions. Sediment microcosm studies may
- of sediment, the deeper sediments tend to harbor anaerobic conditions. Sediment microcosm
   yield variable biodegradation rates as a result of differing microbial populations, ratios of
- 645 sediment/water used, as well as experimental temperature.
- 646
- Two high-quality studies reported aerobic biodegradation rates collected in aqueous test systems
- 648 containing natural sediments. The first study collected top sediment and water from False Creek, a 649 marine inlet in Vancouver, British Columbia, and found BBP to biodegrade with a primary
- biodegradation half-life of 2.9 days (Kickham et al., 2012). Monophthalate ester products all yielded
- half-lives of less than or equal to 3.0 days (<u>Kickham et al., 2012</u>). The second study sampled sediments

from the Zhonggang, Keya, Erren, Gaoping, Donggang and Danshui Rivers in Taiwan, and monitored
the primary biodegradation of a mixture of phthalates in vessels along with a defined nutrient medium
(<u>Yuan et al., 2002</u>). <u>Yuan et al. (2002</u>) reported a mean half-life of 3.1 days for BBP, with a range of 0.5
to 10.5 days.

- 656 657 Anaerobic degradation of BBP in sediments is expected to occur more slowly than aerobic degradation. Two high-quality studies reported anaerobic biodegradation rates collected in natural sediment test 658 659 systems. Yuan et al. (2002) tested sediments from the above listed Taiwanese rivers under anaerobic conditions and found a mean primary biodegradation half-life of 19.3 days, with a range of 9.9 to 25.5 660 days. In three microcosm types run in duplicate containing pond sediments from Ue, Zuion, and Piano 661 662 ponds (Osaka, Japan) and mineral salt medium, primary BBP biodegradation half-lives were shorter at 663 1.5, 2.2, and 1.8 days, respectively (Lertsirisopon et al., 2006). However, there is more uncertainty associated with the experiments reported by Lertsirisopon et al. (2006), as extraction recoveries and the 664 use of control vessels were not reported. 665
- 667 Because of BBP's strong sorption affinity for sediments, biodegradation processes will compete with adsorption processes in sediments. Kickham et al. (2012) describes these interactions with a set of 668 governing equations for the relationships between biodegradation, hydrophobicity (represented by log 669 670  $K_{OC}$  and log  $K_{OW}$ , and organic carbon of a sediment system. For more hydrophobic compounds such as 671 BBP, the apparent biodegradation rate (as measured) may be lower than the inherent or expected 672 biodegradation rate, as adsorption to organic carbon in suspended and settled solids will reduce the fraction of BBP available to microbes for degradation (*i.e.*, the freely dissolved fraction). Among the 673 674 studied diphthalate esters (DPEs), apparent biodegradation rate decreased with increasing log  $K_{OW}$ 675 (Kickham et al., 2012). For aqueous environments not receiving continuous releases of BBP, the fraction 676 of BBP available for biodegradation will increase as the sorption equilibrium shifts towards aqueous 677 phase, re-releasing sorbed fractions of BBP to pore water and water at the water column/sediment 678 boundary. 679
- 680 While the biodegradation rate of BBP in sediments will depend on the microbial community, organic 681 carbon content, and oxygen content, the evidence suggests that the biodegradation rate of BBP in 682 sediment will be on the order of weeks to months.
- 683

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### 684 Biodegradation in Soil

685 No high-quality data sources were identified reporting biodegradation data for BBP in soil. Two medium-quality data sources were extracted for the aerobic biodegradation of BBP in soil, both of which 686 were cited in the European Union Risk Assessment Report for BBP (ECJRC, 2007). The first study 687 observed biodegradation half-lives of 59 and 178 days in soil mixed with two concentrations of wood 688 689 preserving sludge. It was noted that the wood preserving sludge may have been toxic to the microbes, 690 therefore the obtained half-lives are likely overestimations of what may occur in natural soils. The 691 second study reported primary biodegradation rates of 75 percent over 7 days, and 65 percent over 30 692 days in artificial compost media. European Commission, Joint Research Centre (2007) noted that the 693 primary authors did not provide information on the discrepancies between the two reported rates.

- 694
- Because neither of the identified studies are representative of natural soil media, EPA opted to use a
   half-life of 10 days in soil, estimated based on BBP's readily biodegradable designation (U.S. EPA,
- 697 <u>2017</u>). This half-life was used during fugacity modeling (see Sections 3.2 and 5).
- 698

### 699Table 4-1. Summary of Empirical BBP Biodegradation Information

Environmental Conditions	Endpoint Value	Half-life (days) <sup>a</sup>	Reference	Overall Data Quality Ranking
	100% in 14 days (28 °C) for all test conditions in artificial river water containing sludge, pond, and river inoculums; inoculum acclimation not reported; test compound concentration(s) 10 and 40 mg-TOC/L	Sludge inoculum: 2-3 days; river inoculum: 4-6 days; and pond inoculum: 5-6 days (from Figure 1)	Fujita et al. (2005)	High
	93±6% and >99% BBP removal at 5 mg and 20 mg/cycle feed rates, respectively, in SCAS reactor with domestic sewage; HRT 24 hours; acclimation not reported	6.2 and 3.6 hours <sup>b</sup>	Saeger and Tucker (1976)	High
Aerobic primary biodegradation in water (screening studies)	97.2% in 28 days (22 °C) in a shake flask test; inoculum acclimated BBP alone; test compound concentration(s) 20 mg/L	5.43 days <sup>b</sup>	<u>SRC (1983a)</u>	High
	77.7% in 28 days (22 °C) in a shake flask test; inoculum acclimated with mixture of 14 PAEs; test compound concentration(s) 20 mg/L	12.9 days <sup>b</sup>	<u>SRC (1983a)</u>	High
	100% in 7 days (25 °C) in all test vessels of a static flask test in BOD dilution water containing yeast and a settled domestic wastewater inoculum; test compound concentration(s) 5 and 10 mg/L	NA	<u>Tabak et al. (1981)</u>	High
Aerobic ultimate	95.86% in 14 days (ThCO <sub>2</sub> evolution; room temperature) in BOD dilution water with sewage sludge inoculum prepared using the Bunch-Chalmers die-away procedure; test compound concentration(s) 20 mg/L	3.05 days <sup>b</sup>	Saeger and Tucker (1976)	High
biodegradation in water (screening studies)	87.5% in 28 days (22 °C) in shake flask CO <sub>2</sub> evolution test; inoculum acclimated BBP alone; test compound concentration(s) 20 mg/L	9.33 days <sup>b</sup>	<u>SRC (1983a)</u>	High
	42.5% in 28 days (22 °C) in shake flask CO <sub>2</sub> evolution test; inoculum acclimated with mixture of 14 PAEs; test compound	35.1 days <sup>b</sup>	<u>SRC (1983a)</u>	High

Environmental Conditions	Endpoint Value	Half-life (days) <sup>a</sup>	Reference	Overall Data Quality Ranking
	concentration(s) 20 mg/L			
	60–80%, 35–70%, and 30-50% in 14 days (O <sub>2</sub> consumption; 28 °C) with sludge, river, and pond inoculums, respectively, in artificial river water; inoculum acclimation not reported; test compound concentration(s) 10 and 40 mg-TOC/L	Sludge inoculum: 3-7 days; river inoculum: 4 to >14 days; and pond inoculum: 4 to >14 days (from Figure 2)	<u>Fujita et al. (2005)</u>	High
	Monod kinetic parameters: Km 12.8 d <sup>-1</sup> ; Y 0.61; µm 6.95 d <sup>-1</sup> ; Ks 36.25 mg/L; from 6 nutrient solutions containing municipal AS; inoculum acclimation not reported; test compound concentration(s) 100 mg/L	NA	<u>Desai et al. (1990)</u>	High
	50% <sup>14</sup> C-BBP degradation at 3 days, and 80-99% at 5 days (20 °C) in microcosm operated semi- continuously, with water and sediment from Illinois River; test compound concentration(s) 10 and 100 µg/L	1.5 days (10 μg/L test conc.); and 2.2 days (100 μg/L test conc.)	<u>Monsanto (1986a);</u> <u>Adams et al.</u> (1988)	High
Aerobic biodegradation in freshwater microcosms	Half-lives reported for $^{14}$ C-BBP in core chamber microcosms with water and sediment from Lake 34 Busch Wildlife Area; test compound concentration(s) 10 and 1,000 µg/L	Primary half-life: < 2 days; ultimate half- life: 4.7 days	Monsanto (1983c)	High
	BBP degraded to ND, and 5.5 $\mu$ g/L over 5 days (24 °C) at lower and higher test concentrations, respectively in river water die-away test, with water and sediment from Mississippi River; test compound concentration(s) 50.3 and 503 $\mu$ g/L	0.5 (50.3 µg/L); and 1.4 days (503 µg/L) in active river water	Monsanto (1983d)	High
Aerobic biodegradation in sediment	Primary BBP biodegradation rate of $0.24\pm0.07 d^{-1} (14 \text{ °C})$ in a PAE mixture in surface sediment, water and sediment from False Creek, Vancouver; test compound concentration(s) 70 µg/g ww	2.9 days	<u>Kickham et al.</u> (2012)	High
	Half-lives reported for primary BBP biodegradation in a PAE mixture in river sediment in serum bottles with nutrient	0.5 – 10.5 days (mean 3.1 days)	<u>Yuan et al. (2002)</u>	High

Environmental Conditions	Endpoint Value	Half-life (days) <sup>a</sup>	Reference	Overall Data Quality Ranking
	medium; sediments collected from Zhonggang, Keya, Erren, Gaoping, Donggang, and Danshui Rivers, Taiwan; test compound concentration(s) 5 µg/g			
Anaerobic biodegradation in sediment	Half-lives reported for primary BBP biodegradation pond sediments in mineral salt medium; sediments collected from Ue, Zuion, and Piano Ponds, Osaka, Japan; test compound concentration(s) explicitly reported, though were below water solubility	Ue Pond: 1.5 days (1.3-day lag time); Zuion Pond: 2.2 days (no lag); Piano Pond: 1.8 days (1.4-day lag time)	Lertsirisopon et al. (2006)	High
	Half-lives reported for primary BBP biodegradation in a PAE mixture in river sediment in serum bottles with nutrient medium; sediments collected from Zhonggang, Keya, Erren, Gaoping, Donggang, and Danshui Rivers, Taiwan; test compound concentration(s) 5 µg/g	9.9 – 25.5 days (mean 19.3 days)	<u>Yuan et al. (2002)</u>	High
Aerobic biodegradation in soil	Half-lives reported for primary BBP biodegradation in soil and wood preserving sludge; toxicity effects possible; test compound concentration(s) 117 mg/kg	59 and 178 days	<u>ECJRC (2008)</u>	Medium
	75% in 7 days and 65% in 30 days primary biodegradation in artificial compost; test compound concentration(s) 500 $\mu$ g/g	3.5 and 19.8 days <sup>b</sup>	<u>ECJRC (2008)</u>	Medium
Anaerobic biodegradation in soil	No empirical data identified			

<sup>*a*</sup> Half-life values reported by authors unless otherwise noted.

<sup>b</sup> Half-life values calculated assuming first-order kinetics using Equation 3-1. Note that half-lives derived using Equation 3-1 are estimates calculated from a single timepoint rather than a full kinetic study. Therefore, there is greater uncertainty in these calculated half-lives as compared to those directly observed or derived from a full kinetic biodegradation data set.

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### 4.2 Hydrolysis

702 Only one experimental data source describing the hydrolysis of BBP in artificial river water was

identified by the systematic review process (Lertsirisopon et al., 2009). Lertsirisopon et al. (2009)

reported hydrolysis half-lives between 390 and 1,500 days determined in artificial river water at 10  $^{\circ}$ C

and pH values ranging from 5 to 9, with more rapid hydrolysis occurring under both acidic and basic

- conditions as compared to neutral conditions. However, this study was given an overall study quality
- rating of low because the authors employed a BBP concentration of 137.4 mg/L, well over its water
- solubility of 2.69 mg/L (<u>NLM, 2015; Howard et al., 1985</u>). Due to this, EPA deemed the study invalid as
- it is unclear whether homogeneity of BBP was maintained in the test solution for the duration of the
- 710 hydrolysis assessment. Nonetheless, hydrolysis is not expected to be an important transformation 711 pathway in aqueous systems, as biodegradation is expected to occur rapidly in most conditions (see
- pathway in aqueous systems, as biodegradation is expected to occur rapidly in most conditions (see
   Section 4.1). This was demonstrated by Monsanto (1983d) who reported a half-life of 115 days in an
- abiotic (sterilized) control microcosm containing natural Mississippi River water as compared to half-
- 714 lives of 0.5 and 1.4 days in the biologically active microcosms.
- To increase confidence in the contribution of hydrolysis to BBP's fate in aqueous systems, EPA
- 716 leveraged the HYDROWIN<sup>TM</sup> module in EPI Suite<sup>TM</sup> that predicts hydrolysis transformation rates of
- chemicals based on a chemical's structure. HYDROWIN<sup>TM</sup> predicts that BBP will hydrolyze with a
- half-life of 1.4 years at pH 7 and 25 °C, and a half-life of 51 days at pH 8 and 25 °C (U.S. EPA, 2017).
- 719 When compared to other degradation pathways, hydrolysis is not expected to be a significant source of
- 720 BBP degradation under typical environmental conditions.

# 721 **4.3 Photolysis**

Regarding photolysis in the atmosphere, one medium-rated data source was extracted during
systematic review (Peterson and Staples, 2003). For photolysis in water, nine data points from eight
sources were identified and extracted, two data points of which were rated high-quality (Xu et al.,
2009; Monsanto, 1983f).

### 726 *Photolysis in the Atmosphere*

BBP contains chromophores that absorb light at greater than 290 nm wavelength (NCBI, 2020),
therefore, direct photodegradation of BBP may occur in the atmosphere. However, it is expected that
the atmospheric fate and persistence of BBP will be primarily driven by indirect photolysis mediated

- by photolytically induced hydroxyl radicals (·OH). Peterson and Staples (2003), a medium-rated data
   source, reported an atmospheric half-life of 18 hours for BBP based on an ·OH rate constant of
- 1.1049×10<sup>-11</sup> cm<sup>3</sup>/molecule-second, and assuming  $1.0\times10^6 \cdot OH/cm^3$ ; to compare with the predicted
- photolysis half-life estimated by AEROWIN<sup>TM</sup> (discussed below), EPA calculated a half-life of 11.6 hours with the slightly greater radical concentration of  $1.5 \times 10^6 \cdot \text{OH/cm}^3$ . This data was rated as
- 735 medium-quality because it was a secondary source citing property estimation information (Peterson
- 736 <u>and Staples, 2003</u>).
- To increase confidence in the persistence analysis of BBP in the atmosphere, EPA leveraged the
- AEROWIN<sup>TM</sup> module in EPI Suite<sup>TM</sup> that predicts atmospheric transformation rates of chemicals
- based on a chemical's structure and predicted interactions with ozone and common radical-forming (1 0)
- species in the atmosphere (*i.e.*, OH and NO<sub>3</sub>). AEROWIN<sup>TM</sup> predicts that BBP will undergo  $\cdot$  OHmediated indirect photolysis in the atmosphere with a half-life of 0.97 days (23.28 hours) based on an
- restimated  $\cdot$  OH reaction rate constant of  $1.10 \times 10^{-11}$  cm<sup>3</sup>/molecule-second, and assuming a 12-hour day
- 743 with  $1.5 \times 10^6 \cdot \text{OH/cm}^3$  (U.S. EPA, 2017).

### 744 *Photolysis in Surface Water*

- One of the two high-quality data sources extracted with information on the photolysis rate of BBP in
- aqueous systems reported the indirect photolysis of BBP in a titanium(IV) dioxide (TiO<sub>2</sub>)/UV
- 747 photocatalysis system (16 black/blue fluorescent UV lamps operating at 250 nm, 8-watt maximum

- 748 output) (Xu et al., 2009). Because the TiO<sub>2</sub>/UV system is not representative of natural surface waters,
- this study was neither selected for use to represent the photolytic fate of BBP, nor for use in the fate
- analysis of BBP in aquatic environments. The second high-quality data source reported a direct
- 751 photolysis rate of 1 percent over 28 days (total natural sunlight irradiation time approximately 251
- hours) at a BBP test concentration of 1.051 mg/L in purified (MilliQ) water (Monsanto, 1983f).
- 753 Because biodegradation is expected to be the primary transformation process driving BBP's fate in
- aqueous systems (see Section 4.1), EPA did not further consider photolysis in water in its fate analysis.
- 755

# 756 **5 PARTITIONING, TIER I, AND TIER II ANALYSES**

### 757

# 5.1 Identification and Selection of Partition Coefficients for BBP

The log K<sub>OW</sub> value used for BBP in the present Tier I analysis was the same selected value as discussed in Section 2.2.7 and extracted from (NLM, 2015). No data were identified reporting empirical octanol:air (log K<sub>OA</sub>) values for BBP. EPA leveraged the KOAWIN<sup>TM</sup> model as part of EPI Suite<sup>TM</sup> to obtain an estimated log K<sub>OA</sub> value of 9.27 (U.S. EPA, 2017).

762 763 Two data sources reported modeled (estimated) values for the air:water partition coefficient. Lu (2009) developed a QSPR model for the prediction of partitioning coefficients for a set of 53 phthalates, 764 765 including BBP. A log  $K_{AW}$  of -3.76 was predicted for BBP, indicating a strong affinity for aqueous phase over vapor phase. The same study also estimated a log K<sub>OA</sub> value of 8.98, in good agreement with 766 the value of 9.27 modeled using KOAWIN<sup>TM</sup>, as discussed above. The second study estimated a log 767 K<sub>AW</sub> of -4.08 using the three-solubility approach, calculating K<sub>AW</sub>, K<sub>OA</sub>, and K<sub>OW</sub> from ratios of 768 "apparent-solubilities" (concentrations) of phthalates in air, water, and octanol and their relationships 769 770 (regression analysis) to respective molar volumes (Cousins and Mackay, 2000). The same method predicted a log  $K_{OW}$  of 4.70, and a log  $K_{OA}$  of 8.78, in good agreement with the selected empirical log 771 772 K<sub>OW</sub> (4.73; (NLM, 2015)) and estimated log K<sub>OA</sub> (9.27, (U.S. EPA, 2017)) for BBP, respectively. These estimated log K<sub>AW</sub> values are also consistent with the magnitude of the selected HLC for BBP of 773 774  $7.61 \times 10^{-7}$  atm·m<sup>3</sup>/mol, indicating a slight possibility of volatilization from wet surfaces (Elsevier, 2019) 775 (see Section 2.2.8).

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7	7	7

Measurement Conditions	Endpoint Value	Reference	Overall Data Quality Ranking
Organic Carbon:Water Partition Coefficient	Log K <sub>OC</sub> : 3.38, 3.43, 3.46, and 3.52 L/kg in Spinks soil, and 4.01 in Drummer soil (mean = $3.56$ ) tested with MilliQ water; soil mean %OC: 2.9%	Monsanto (1983b)	High
(Log K <sub>oc</sub> ) (soil)	Log K <sub>OC</sub> : 4.23 L/kg with composite soil from Broome County, NY; soil mean %OC: 1.59%	Russell and Mcduffie (1986)	High
Organic Carbon:Water Partition Coefficient (Log K <sub>OC</sub> ) (sediment)	Log K <sub>OC</sub> : 5.74, 5.76, 5.78, 5.79, and 5.81 L/kg (mean = $5.78$ L/kg) with five marine sediment samples from Victoria Harbor, Hong Kong, and artificial saltwater mixtures; pH = $7.5$ ; sediment mean %OC: 1.66%	<u>Xu and Li (2009)</u>	High

### Table 5-1. Summary of Empirical Log $K_{OC}$ Information for BBP

Measurement Conditions	Endpoint Value	Reference	Overall Data Quality Ranking
	Log K <sub>OC</sub> : $5.52\pm0.17$ and $6.21\pm0.17$ L/kg (mean = $5.87$ L/kg) determined with glass fiber filtration and C <sub>18</sub> disk adsorption, respectively, in marine sediment and water samples from False Creek Harbor, Vancouver; sediment mean %OC: 2.80%	Mackintosh et al. (2006)	High
Organic Carbon:Water Partition Coefficient (Log K <sub>OC</sub> ) (suspended particulate matter [SPM])	Log $K_{OC}$ : 5.09, 5.19, and 5.91 L/kg (mean = 5.40 L/kg) with freshwater suspended particulate matter and water samples from 20 sites in Lake Chaohu, China collected in summer, autumn and winter, respectively; suspended particulate matter measured but not reported	<u>He et al. (2019)</u>	High
	Log K <sub>OC</sub> : $6.38\pm0.29$ and $6.75\pm0.25$ L/kg (mean = $6.57$ L/kg) determined with glass fiber filtration and C <sub>18</sub> disk adsorption, respectively, with marine suspended particulate matter and water samples from False Creek, Vancouver; suspended particulate matter mean %OC: $40.0\%$	Mackintosh et al. (2006)	High

### 778

788

779 Sixteen data sources were identified reporting adsorption information for BBP from both field and 780 laboratory studies, ten of which were given an overall quality rating of high. EPA considered only the high-quality adsorption studies when performing the present partitioning analysis. Five of the ten 781 782 identified high-quality studies were excluded from use in this analysis due to the following reasons: 1) 783 irrelevant system to inform environmental partitioning (landfill media; (Asakura et al., 2007)); 2) low 784 detection frequency and therefore statistical power from field measurements (Vitali et al., 1997); 3) no 785 organic carbon measurements taken of solid phase (Li et al., 2016b; Li et al., 2015); 4) test method did not yield a K<sub>OC</sub> or equivalent sorption value that may be used in subsequent modeling (Sayyad et al., 786 787 2017).

789 Three of the remaining high-quality studies reported BBP adsorption coefficients in aqueous systems. 790 He et al. (2019) reported log K<sub>OC</sub> values for BBP adsorption to suspended particulate matter (SPM) in 791 freshwater Lake Chaohu, China, over three seasons. The authors reported mean log  $K_{OC}$  values 792 2.09±0.67 L/g in summer samples, 2.19±0.87 L/g in autumn samples, and 2.91±0.82 L/g in winter 793 samples. Authors note that lack of means to verify consistent equilibrium among the dispersed sampling 794 sites may have contributed to the obtained measurement variances (He et al., 2019). However, shifting 795 of equilibrium due to volatilization is not expected to be relevant for BBP given its low tendency to 796 volatilize from surface waters, as discussed above.

797
798 A similar study investigated the log K<sub>OC</sub> of BBP associated to both suspended particulates and surface
799 sediments collected from four locations in False Creek Harbor, Vancouver (Mackintosh et al., 2006).
800 The authors distinguished between log K<sub>OC</sub> values derived using "operational" water concentrations and
801 "true" freely dissolved water concentrations. The log K<sub>OC</sub> values for BBP adsorption to suspended

802 particulates were reported to be 6.38±0.29 and 6.75±0.25 using operational water concentrations and 803 true freely dissolved concentrations, respectively (Mackintosh et al., 2006). The log K<sub>OC</sub> values for BBP 804 adsorption to surface sediments were reported to be  $5.52\pm0.17$  and  $6.21\pm0.17$  using operational water 805 concentrations and true freely dissolved concentrations, respectively (Mackintosh et al., 2006). These 806 results indicate three important patterns: 1) BBP tends to adsorb more readily to suspended solids in the 807 water column as compared to particulates that settle to the sediment layer, likely due to structural 808 differences of the particle fractions (e.g., density, surface area) between the two solid phase types; 2) log 809 Koc values derived using filtration methods prior to extracting the water phase will yield lower log Koc values which may contribute to underestimations of the tendency of the chemical to remain dissolved in 810 811 true aqueous phase, affecting subsequent exposure analyses; and 3) the study yielded greater log  $K_{OC}$ 812 values than determined in the freshwater system by He et al. (2019), evidence that  $\log K_{OC}$  values of 813 highly hydrophobic compounds such as BBP are likely to be very sensitive to salinity/salting out effects.

814

815 Xu and Li (2009) also reported empirical log  $K_{OC}$  values collected representative of marine conditions 816 with sediments collected from five locations in Victoria Harbor, Hong Kong. The authors investigated 817 the effects of sediment organic matter content, temperature, and water salinity on the  $\log K_{OC}$  measured 818 with the collected sediment and artificial marine water. Xu and Li (2009) observed that equilibrium in 819 the test systems was reached rapidly, with greater than 59 percent of sorption occuring within the first 30 820 minutes of the test, and equilibrium reached within 6 hours. The reported  $K_{OC}$  ranged from 555 to 640 821 L/g (mean 598±33 L/g) with unadjusted sediment, temperature, and salinity. Increasing the salinity of 822 the artificial marine water increased the fraction of BBP adsorbed to the sediments, confirming the presence of a salting out effect. Temperature was found to be inversely related to  $K_{OC}$  (Xu and Li, 2009). 823 824 Overall, measured  $K_{OC}$  of BBP adsorbed to particulates and sediments in aqueous systems is largely 825 sensitive to the salinity of the system, as well as extraction/filtration techniques which may differ 826 depending on the composition of suspended particulates in the water column.

827

Two high-quality data sources were identified reporting log Koc values for BBP measured with soil. In a 828 829 screening adsorption test, Monsanto (1983b) measured adsorption coefficients of 70, 57, 79, and 64 in Spinks soil, and 350 in Drummer soil when tested with MilliQ water as the aqueous phase. When 830 831 normalized to the reported percent organic carbon (%OC) of 2.4 percent in Spinks soil and 3.4 percent 832 in Drummer soil, these coefficients may be represented as log K<sub>OC</sub> values of 3.38, 3.43, 3.46, and 3.52 833 L/kg in Spinks soil, and 4.01 in Drummer soil (overall mean = 3.56). The second soil log K<sub>OC</sub> value was 834 measured using a composite soil from Broome County, NY 4.23 L/kg measured in a flask test system 835 (Russell and Mcduffie, 1986). While lower in magnitude, the log  $K_{OC}$  values collected using soil media agree well with those collected with sediment media indicating that BBP will sorb appreciably to 836 837 organic matter in solid media. The greater log K<sub>OC</sub> values in sediment systems than in soil systems) is 838 likely due to differences in solid phase composition and organic matter, as well as differences in 839 aqueous phases used. To represent a range of environmental conditions, the average ( $\log K_{OC} = 4.86$ 840 L/kg) of mean study log K<sub>OC</sub> values collected using soils (Russell and Mcduffie, 1986; Monsanto, 1983b) and sediments (Xu and Li, 2009; Mackintosh et al., 2006) was used during Tier I and Tier II 841 analyses, results described below. 842

# **5.2 Results of Tier I Partitioning Analysis**

To be able to understand and predict the behaviors and effects of BBP in the environment, a Tier I analysis will determine whether an environmental compartment (*e.g.*, air, water, etc.) will accumulate BBP 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 BBP is to consider partitioning values which indicate the potential for a substance to favor one compartment over another. The selected values to represent the partitioning behavior of BBP among media types are

850 presented in Table 5-2.

851

### 852 Table 5-2. Partition Coefficients Selected for Tier I Partitioning Analysis of BBP

Partition Coefficient	Value <sup>a</sup>	Log Value	Source(s)	Predominant Phase
Octanol:Water (K <sub>OW</sub> )	5.37E04	4.73	<u>NLM (2015)</u>	Organic Carbon
Organic Carbon:Water (K <sub>OC</sub> )	7.24E04	4.86	Average of mean study values (n = 4) reported in soil ( <u>Russell and Mcduffie, 1986;</u> <u>Monsanto, 1983b</u> ) and sediment media ( <u>Xu</u> <u>and Li, 2009; Mackintosh et al., 2006</u> )	Organic Carbon
Octanol:Air (K <sub>OA</sub> )	1.85E09	9.27	$KOAWIN^{TM} \underline{U.S. EPA (2017)}$	Organic Carbon
Air:Water (K <sub>AW</sub> )	1.2E-04	-3.92	Average of values (n = 2) from <u>Cousins and</u> <u>Mackay (2000)</u> and <u>Lu (2009)</u>	Water
<sup><i>a</i></sup> Measured unless otherwise noted.				

### 853

Based on the magnitude of log K<sub>OC</sub> and log K<sub>OA</sub> values identified for BBP, BBP 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 BBP.

857 858 BBP is a liquid at environmental temperatures with a melting point of  $-35^{\circ}C$  (NLM, 2015) and a vapor 859 pressure of  $8.25 \times 10^{-6}$  mm Hg at 25 °C (Howard et al., 1985). Based on the magnitude of its vapor pressure, BBP will exist predominantly in the particulate phase with potential to exist in the vapor 860 861 (gaseous) phase in the atmosphere based on the measured vapor pressure. The octanol:air coefficient (K<sub>OA</sub>) indicates that BBP will favor the organic carbon present in airborne particles. Based on its 862 physical and chemical properties and short half-life in the atmosphere ( $t_{1/2} = 0.97$  days), BBP was 863 assumed to not be persistent in the air. The AEROWIN<sup>™</sup> module in EPI Suite<sup>™</sup> estimates that a fraction 864 of BBP could be sorbed to airborne particulates and these particulates may be resistant to atmospheric 865 866 oxidation. Monitoring studies have detected BBP in ambient air, settled house dust, indoor air samples and in indoor particulate phase air samples (Kubwabo et al., 2013; Wang et al., 2013; ECJRC, 2007; 867 868 EC/HC, 2000).

869

The air:water partitioning coefficient ( $K_{AW}$ ) indicates that BBP will favor water over air. With a water solubility of 2.69 mg/L at 25 °C, BBP is expected to be slightly soluble in water (<u>Howard et al., 1985</u>). BBP in water will partition to suspended organic material present in the water column based on BBP's low water solubility and high partition coefficients to organic matter. In addition, total seawater sample concentrations of BBP measured in False Creek ranged from 2 to 6 ng/L; the freely dissolved fraction concentrations ranged from 0.97 to 3.28 ng/L and the suspended particulate fraction concentration ranged from 1,250 to 5,650 ng/g dry weight (dw) (<u>Mackintosh et al., 2006</u>).

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878

# 5.3 Results of Tier II Partitioning Analysis and Fugacity Modeling

The approach described by <u>Mackay et al. (1996)</u> using the Level III Fugacity model in EPI Suite<sup>TM</sup> (LEV3EPI<sup>TM</sup>) was used for this Tier II analysis. LEV3EPI is described as a steady-state, nonequilibrium 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). BBP's physical and chemical properties were taken directly from

884 Section 2.1, and additional method information for the Tier II analysis and fugacity modeling are 885 described in Section 3.3.

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887 The results of Level III Fugacity modeling are presented in Figure 5-1. The fugacity results suggest that 100 percent of releases to soil will remain in soil; 58 percent of releases to water will remain in water 888 889 with about 41.9 percent partitioning to sediments; and 60.6 percent of releases to air will end up in soil with another 4.51 percent in water and 31.7 percent remaining in air. Based on BBP's environmental 890 891 half-lives, partitioning characteristics, and the results of Level III Fugacity modeling, BBP is expected to be found predominantly in soil and to a lesser extent water and sediment. It should be noted that these 892 893 estimations are based on steady-state, non-equilibrium conditions (*i.e.*, continuous releases) Therefore, 894 actual concentrations in environments receiving a single, pulse input of BBP may be low due to the 895 anticipated low persistence potential of BBP, primarily mediated by biodegradation processes (see 896 Section 4.1).

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> 100 90 80 70 60 50 40 30 20 100 Equal Releases 100% Air Releases 100% Air Releases 100% Soil Releases

> > Air Water Soil Sediment

Figure 5-1. EPI Suite<sup>TM</sup> Level III Fugacity Modeling Graphical Result for BBP

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# 904 6 MEDIA ASSESSMENTS

905 BBP has been reported to be present in the atmosphere, aquatic environments, and terrestrial 906 environments. Once in the air, BBP will be most predominant in the organic matter present in airborne particles and expected to have a short half-life in the atmosphere. Based on the physical and chemical 907 908 properties, BBP in indoor air is likely to partition to house dust and airborne particles and is expected to 909 have a longer half-life compared to ambient (outdoor) air. BBP present in surface water is expected to mostly partition to aquatic sediments. BBP is expected to have an aerobic biodegradation half-life 910 911 between about 0.5 to 35 days. In terrestrial environments BBP has the potential to be present in soils and 912 ground water but is likely to only be slightly mobile in both media types. In soils, BBP is expected to be 913 deposited via air deposition and land application of biosolids. BBP in soils is expected to have a half-life

on the order of days to weeks and have low bioaccumulation potential and biomagnification potential in

915 terrestrial organisms. BBP may arrive in groundwater via infiltration of wastewater effluent and landfill

916 leachates, though it is not likely to be persistent in most groundwater/subsurface environments.

# 917 **6.1 Air and Atmosphere**

BBP is a liquid at environmental temperatures with a melting point of -35°C (Haynes, 2014b) (NLM, 918 2015) and a vapor pressure of  $8.25 \times 10^{-6}$  mmHg at 25 °C (<u>Howard et al., 1985</u>). Based on its physical 919 and chemical properties and short half-life in the atmosphere ( $t_{1/2} = 0.75 - 0.97$  days via indirect 920 photodegradation) (U.S. EPA, 2017; Peterson and Staples, 2003), BBP is not expected to be persistent in 921 the ambient air. The AEROWIN<sup>TM</sup> module in EPI Suite<sup>TM</sup> estimated a log K<sub>OA</sub> of 9.2, which suggests 922 923 that BBP will have a strong affinity for organic matter in air particulates. The physical and chemical 924 properties of BBP suggest that it has the potential to undergo dry and wet deposition but that its 925 transport in air will be mediated by indirect photodegradation (Zeng et al., 2010; Peters et al., 2008; Xie 926 et al., 2005; Parkerton and Staples, 2003).

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934

928 Phthalate esters have been frequently detected in the atmosphere and indoor air. Their worldwide

presence in air has been documented in the gas phase, suspended particles, and dust (<u>Net et al., 2015</u>).

BBP is expected to be more persistent in indoor air than in ambient (outdoor) air due to the lack of

natural chemical removal processes, such as solar photochemical degradation. Based on its short half-

life in the atmosphere, BBP is not expected to be persistent in atmospheric air under normal

933 environmental conditions.

### 6.1.1 Ambient Air

Despite its half-life in air of 0.75 to 0.97 days, BBP has been frequently measured at low concentrations 935 in ambient air. For instance, two studies reported gas phase concentrations of BBP in ambient air of 0.01 936 to 0.04 ng/m<sup>3</sup> over the North Sea (Xie et al., 2005) and 0.017 to 0.068 ng/m<sup>3</sup> over the Arctic (Xie et al., 937 2007). These two studies also reported that 44 to 75 percent of BBP in the air was associated with 938 939 suspended particles and that in the North Sea there was a net deposition of BBP from ambient air into 940 water (Xie et al., 2007; Xie et al., 2005). Additionally, two studies conducted at day care centers in the U.S. reported BBP concentrations ranging from less than 1 to 733 ng/m<sup>3</sup> in outdoor air (Wilson et al., 941 2003; Wilson et al., 2001). Other studies conducted outside the U.S. measured concentrations of BBP in 942 ambient air with a range of 0.02 to 17 ng/m<sup>3</sup> in Sweden (Cousins et al., 2007); 1.51 to 3.6 ng/m<sup>3</sup> in air 943 over the Mediterranean Sea (Romagnoli et al., 2016); and range of 4.7 to 12.1 ng/m<sup>3</sup> in the vapor phase 944 945 and 14.5 to 12.7 mg/kg sorbed to particles in France (Teil et al., 2006). Overall, the data suggest that BBP is likely to be present in ambient air at low concentrations and a large percentage will be associated 946 947 with particulates.

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### 6.1.2 Indoor Air and Dust

949 EPA identified several data sources reporting the presence of BBP in indoor air and dust within the 950 United States. Wilson et al. (2001) measured samples of indoor air and dust from ten daycare centers in 951 North Carolina. BBP was detected in all air and dust samples above the method detection limit with a mean concentration of 100  $ng/m^3$  and range of 108 to 404  $ng/m^3$  in air samples, and a mean 952 953 concentration of 67.7 mg/kg and range of 15.1 to 175 mg/kg in dust samples. Another study conducted 954 in residential and office buildings in Massachusetts found BBP in dust samples ranging from 12.1 to 524 955 mg/kg, with a mean of 117 mg/kg and a detection frequency of 100 percent (Rudel et al., 2001). 956 Additionally, Dodson et al. (2015) reported BBP concentrations in house dust from California of below

- 957 the detection limit to 330 mg/kg, with a median of 19 mg/kg.
- 958

959 EPA also identified several data sources reporting the presence of BBP in indoor air and dust outside the 960 United States. Das et al. (2014) measured concentrations of phthalates in indoor air and dust samples 961 from Jawaharlal Nehru University (JNU), a campus with low industrial activity, and Okhla, a city with 962 high industrial activity related to the use of phthalates. The study reported that BBP concentrations in 963 outdoor air, indoor air, and indoor dust were higher in Okhla than JNU, demonstrating that industrial 964 activities may lead to higher exposures near an emitting facility. Another study conducted using 965 Swedish house dust reported an average BBP concentration in total dust of 0.96 µg/mg sedimented dust, 966 with  $1.23 \times 10^{-3}$  mg/kg associated with the organic fraction of the dust (Oie et al., 1997). In a study 967 conducted in Japan. BBP was found to range from below the detection limit to  $26.6 \text{ ng/m}^3$  in air, and 968 from below the detection limit to 52.1 mg/kg indoor dust in residential houses (Kanazawa et al., 2010). 969 Another study measuring BBP concentrations in house dust from German households found 970 concentrations ranging from below the detection limit to 767 mg/kg, with a median of 15.2 mg/kg (Abb 971 et al., 2009). Wang (2013) also reported higher concentrations of BBP in indoor dust compared to 972 outdoor dust, at average concentrations of 8.22 mg/kg and 0.72 mg/kg, respectively. Further, BBP was 973 found to be a minor phthalate at 3 to 27 percent of the total phthalate concentration in particulate matter 974 in indoor spaces in Norway (Rakkestad et al., 2007). These data suggest that BBP is likely to be found in 975 indoor dust and air and at higher concentrations in indoor air compared to outdoor ambient air.

### 976 **6.2 Aquatic Environments**

### 6.2.1 Surface Water

BBP 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. BBP has been detected in
surface waters, though generally at lower concentrations than other common co-occurring phthalates
such as DBP and DEHP (Grigoriadou et al., 2008; Mackintosh et al., 2006; Yuan et al., 2002; Preston
and Al-Omran, 1989).

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977

984 The principal properties governing the fate and transport of BBP in surface water are water solubility 985 (2.69 mg/L; (NLM, 2015)), air:water partitioning coefficient (log  $K_{AW} = -3.92$ ; mean of values from Cousins and Mackay (2000) and Lu (2009), and organic carbon partitioning coefficients (log  $K_{OC}$  = 986 987 5.52-6.21 in sediments (Xu and Li, 2009; Mackintosh et al., 2006), and 5.09-6.75 L/kg to suspended particulate matter (He et al., 2019; Mackintosh et al., 2006)). Due to the Henry's Law constant, HLC 988  $(7.61 \times 10^{-7} \text{ atm} \cdot \text{m}^3/\text{mol} (\text{Elsevier}, 2019))$  of BBP, volatilization is not expected to be a significant 989 990 transport pathway. A partitioning analysis of BBP released to water estimates that about 39 percent of 991 the BBP released to water will partition to sediments and about 61 percent will remain in surface water 992 as described in Section 5 above. The same fugacity model run predicted that 5.26 percent of the total 993 BBP released to water will remain adsorbed to suspended particulate matter (U.S. EPA, 2017). Based on 994 the organic carbon partition coefficients, BBP remaining in the water column will readily adsorb to 995 suspended particulate matter to varying degrees, as discussed in the subsequent paragraph (mean SPM 996 log  $K_{OC}$  = 5.99; see Table 5-1). Free/unbound BBP is expected to biodegrade rapidly in most aquatic 997 environments (see Section 4.1 and Table 4-1) and thus is not expected to persist in surface water except 998 at areas of continuous release, such as a surface water body receiving discharge from a municipal 999 wastewater treatment plant, where rate of release exceeds the rate of biodegradation.

1000

1001 There is a range in the expected relative distribution of BBP between freely dissolved and particulate-1002 associated (SPM) fractions that have been demonstrated to vary with salinity, temperature, and BBP 1003 concentration. First, salinity is an important driver of BBP sorption to solids in aqueous systems, as the

1004 freely dissolved fraction decreases consistently with increasing salinity (0-35 ppt), indicating a salting 1005 out effect (Xu and Li, 2009). The salting out effect may help to explain the order of magnitude 1006 difference between the  $K_{OC}$  values determined with SPM in a freshwater system (mean log  $K_{OC} = 5.40$ 1007 L/kg; (He et al., 2019)) and a marine system (mean log  $K_{OC} = 6.57$  L/kg; (Mackintosh et al., 2006). Xu 1008 and Li (2009) also indicated that the fraction of BBP sorbed to solids was inversely related to 1009 temperature within the tested range (24.9-34.9 °C). These effects are also discussed in Section 5. Last, 1010 when concentrations above the water solubility were employed in biodegradation studies, authors took 1011 note of possible heterogeneous spatial distribution of BBP in the aqueous phase, and that dispersion of 1012 BBP within the water column may limit biodegradation rates due to lack of complete mixing (Monsanto, 1013 1983e). For all instances where the partitioning equilibrium is shifted towards greater sorption of BBP to 1014 solids, it is expected that overall biodegradation of total BBP in the water column will decrease, with 1015 lower concentrations of freely dissolved BBP being bioavailable.

1016

1017 The available data sources reported the presence of BBP and other phthalates in surface water samples

1018 collected from rivers and lakes globally. <u>Preston and Al-Omran (1989)</u> explored the presence of

- phthalates within the River Mersey Estuary (northwest England) reporting the presence of BBP freely
   dissolved in the water phase at concentrations below the limit of detection up to 0.135 µg/L.
- $\frac{\text{Grigoriadou et al. (2008)}{\text{Grigoriadou et al. (2008)}}$  reported the presence of DIBP, DBP, BBP and DEHP on lake water samples collected near the industrial area of Kavala, Greece. The detected concentrations of BBP in lake water ranged from 0.083 to 58.200 µg/L (Grigoriadou et al., 2008). False Creek Harbor (Vancouver, British Columbia) total (dissolved and SPM-sorbed) water concentrations of BBP ranged from 1.89 to 6.41 ng/L with the operationally dissolved (<0.45 µm) fraction concentrations ranging from 0.97 to 3.28 ng/L
- and the suspended fraction concentrations ranging from 1,250 to 5,650 ng/g dw. These data show higher concentrations of BBP in the SPM than in the operationally dissolved phase, which is to be expected given the  $K_{OC}$  and partitioning analysis (see Section 5) results for BBP.
- 1029

1030 Concentrations and detection frequencies for BBP in surface waters measured in the U.S. are generally 1031 low. BBP measured in the Nanticoke River, MD (a tributary of the Chesapeake Bay) reported a 1032 detection frequency of 0 percent with a limit of detection (LOD) of 1 µg/L (Hall et al., 1985). Similarly, 1033 Burgess & Niple (1981) detected BBP in one of three sites sampled in Scippo Creek, OH, though the 1034 detection was below the limit of quantification (LOQ) of 10 µg/L. In monitoring of rivers in the U.S., 1035 Gledhill et al. (1980) reported an overall detection frequency of 66% (LOD  $0.2 \mu g/L$ ), with no 1036 detections reported for San Francisco Bay, and the most detections found in the Mississippi River in St. 1037 Louis, MO (range of  $0.30-2.4 \mu g/L$ ; n = 10).

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1039 More recent monitoring studies conducted in the U.S. are either consistent with the above reported 1040 studies in terms of detection frequency or have employed more sensitive analytical techniques to resolve 1041 BBP concentrations in the ng/L range. Coiner et al. (2010) reported a 0 percent detection rate of BBP in 1042 streams receiving water from draining munitions firing points and impact areas, Fort Riley, Kansas 1043 (LOD range from 10.2 to 13.3 µg/L). In a survey of the Delta (Sacramento) and Bay Area, CA, Oros et al. (2003) reported a detection frequency of 20 percent, with no detections in the Delta, Central Bay, 1044 1045 South Bay or Golden Gate areas, and a total water concentration of 327 ng/L in the North Bay. To 1046 contrast, the median and maximum total BBP concentrations were 67 ng/L and max 144 ng/L in Eleven 1047 Point River (100% detection), and 44 ng/L and max 351 ng/L in the North Fork of White River (93% 1048 detection), respectively.

1049 6.2.2 Sediments 1050 The fate of BBP in sediments is largely governed by its affinity for organic carbon in sediment media, as 1051 well as its readily biodegradable nature. Based on a mean of empirical sediment  $\log K_{OC}$  values of 5.83 (Xu and Li, 2009; Mackintosh et al., 2006), BBP will readily partition to the organic matter present in 1052 1053 soils and sediment when released into aquatic environments. With continuous releases to water, the Level III Fugacity Model in EPI Suite<sup>TM</sup> (U.S. EPA, 2017) predicts that close to 42 percent of the BBP 1054 1055 will partition to the sediment compartment, and 6.38 percent of the total emissions to water will 1056 biodegrade in the sediment compartment, (Section 5). Full fugacity model outputs are provided in 1057 Section 5.3. 1058

BBP is expected to biodegrade rapidly in most aquatic environments (see Section 4.1). Empirical halflives range from 0.5 days (aerobic) to 25.5 days (anaerobic) in river sediments (Yuan et al., 2002). However, it has been suggested that phthalate esters that inherently biodegrade in sediments have increased persistence in sediments with increasing sorption potential to sediments, as sorbed fractions are less bioavailable to microbial degradation (Kickham et al., 2012). This suggests that BBP could persist longer in subsurface sediments than in the water column, and longer than suggested by the controlled laboratory biodegradation studies as discussed in Section 4.1.

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1067 The BBP partitioning to aquatic sediments is consistent with the available monitoring data sources1068 containing information on BBP in river sediment samples.

1069

1070 Several international studies have reported the presence of BBP in sediment samples at concentrations 1071 ranging from below the limit of detection to 150 ng/g dw (Cheng et al., 2019; Tang et al., 2017; Preston 1072 and Al-Omran, 1989). Additionally, several studies conducted in the U.S. monitored for, but did not 1073 detect BBP in any of their sediment samples. These studies were conducted in the Jiulong River, 1074 Southeast China (LOD between 1 and 5  $\mu$ g/kg; (Li et al., 2017)); Green Pond Brook and Bear Swamp 1075 Brook, NJ (reporting limit 200  $\mu$ g/kg; (Storck and Lacombe, 1997)), and Fort Bragg, NC (LOD 500 1076  $\mu$ g/kg in streams near a demolished asphalt plant; (Campbell, 1997)).

Lin et al. (2003) measured phthalate concentrations in sediments and striped perch in four locations in
False Creek Harbor, Vancouver. Mean concentrations of all the monitored phthalate esters ranged from
2.0 to 3.6 mg/kg dw across the four sediment sample locations. While precise concentrations were not
explicitly provided, the authors stated that the concentrations of dimethyl phthalate (DMP), diethyl
phthalate (DEP), DIBP, DBP, and BBP represented about 5 percent of the total concentration of the
monitored phthalate esters.

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1085 Additional monitoring in the U.S. has shown large ranges in BBP sediment concentrations. Gledhill et 1086 al. (1980) detected BBP in three of nine sampling locations in surveys of rivers in the U.S.: mean 1087 concentrations and detection frequencies were reported as 567 (100%), 400 (100%), and 100 (25%) ng/g 1088 ww in the Upper Saginaw, Lower Saginaw, and Missouri Rivers, respectively. The other six locations were below the detection limit of 100 ng/g ww (moisture content not reported) (Gledhill et al., 1980). In 1089 1090 coastal surface waters along coastal Washington state, BBP presence was reported as below method 1091 reporting limits in freshwater (LOQ 0.51 µg/L), SPM, and sediment samples (LOQ range 30–106 µg/kg 1092 dw for SPM and sediments), with one tentatively identified case in marine sediments (3% detection 1093 frequency) (WA DOE, 2022), Papoulias and Buckler (1996) reported sediment concentration ranges of 1094 less than 180 to 15,000  $\mu$ g/kg, less than 240 to 16,000  $\mu$ g/kg, and less than 18 to 3,000  $\mu$ g/kg in Buffalo 1095 River, Indiana Harbor, and Saginaw River, respectively as part of the Assessment and Remediation of

1096 Contaminated Sediments Program operated by the Great Lakes Program Office. The wide variance in 1097 monitored BBP in sediments is likely due to a combination of varying biodegradation capacities by 1098 sampling site, extraction and analytical method sensitivity, and a wide range of collection dates and 1099 therefore potential sources and transformation times relative to time of release.

### 1100 **6.3 Terrestrial Environments**

### 1101 **6.3.1 Soil**

BBP is expected to be deposited to soil via two primary routes: application of biosolids in agricultural applications or sludge drying applications; and atmospheric deposition. Based on its HLC of  $7.61 \times 10^{-7}$ atm·m<sup>3</sup>/mol and vapor pressure of  $8.25 \times 10^{-6}$  mmHg, BBP is not likely to volatilize significantly from soils.

BBP is expected to show strong affinity for sorption to soil and its organic constituents based on a log
K<sub>OC</sub> of 4.86 (Section 5), and a log K<sub>OW</sub> of 4.73 (<u>NLM, 2015</u>). Thus, BBP is expected to have slow
migration potential in soil environments.

1110

1106

1111 EPA did not identify any high-quality studies reporting biodegradation in soils; because of this, EPA

opted to use a half-life of 10 days in soil, approximated based on BBP's readily biodegradable designation, for the purposes of this evaluation (U.S. EPA, 2017) (Section 4.1). Overall, EPA has

1114 moderate confidence that BBP will biodegrade rapidly in soil.

1115

1116 EPA identified 17 studies and reports conducted in the U.S. measuring BBP in soils. Wilson et al.

1117 (2001) measured BBP in soil from outdoor play areas at five daycare centers in North Carolina in spring

1118 1997 and found concentrations ranging from 4.11 to  $1.02 \times 10^2 \,\mu$ g/kg. In a follow-up study, two of the

1119 same daycare centers found concentrations of less than 2.0 to  $64 \mu g/kg$ , with BBP only detected in two

1120 of the four samples (<u>Wilson et al., 2003</u>). EPA also evaluated fifteen studies submitted under TSCA

section 8(d) by automobile, chemical, and aerospace manufacturing facilities in the 1980s and 1990s (Campbell, 1997; ENSR, 1996a, b, 1995; Ecology and Environment, 1992; ERM-Northeast, 1992;

1123 Hargis & Montgomery Inc, 1992; Geraghty & Miller Inc, 1991; Malcolm Pirnie Inc, 1991;

1124 <u>Westinghouse Electric Corporation, 1991; Geraghty & Miller Inc, 1990; Westinghouse Electric</u>

1125 Corporation, 1990; Bechtel Environmental, 1988; Dames & Moore, 1988; Hargis & Montgomery Inc,

1126 <u>1984</u>). Only two of these studies reported a measurable soil concentration of BBP ranging from 12 to

1127 690  $\mu$ g/kg (<u>ERM-Northeast, 1992</u>; <u>Bechtel Environmental, 1988</u>). All other samples from these studies 1128 were either below the detection or quantification limit.

were either below the detection or quantification in

### 1129 **6.3.2 Biosolids**

1130 Sludge is defined as the solid, semi-solid, or liquid residue generated by wastewater treatment processes. 1131 The term "biosolids" refers to treated sludge that meet the EPA pollutant and pathogen requirements for 1132 land application and surface disposal and can be beneficially recycled (40 CFR part 503) (U.S. EPA, 1133 1993). Typically, chemical substances with very low water solubility and high sorption potential are 1134 expected to be sorbed to suspended solids and efficiently removed from wastewater via accumulation in sewage sludge and biosolids. As described in Section 7.2, sorption to sewage sludge can be a major 1135 removal mechanism of BBP during wastewater treatment. Based on the STP module in EPI Suite<sup>TM</sup>, 1136 1137 only 18.31 percent of BBP present in wastewater is expected to be accumulated in sewage sludge and 1138 discharged in biosolids (U.S. EPA, 2017).

1139

A survey of POTW in the US conducted by EPA reported BBP concentrations in undigested combined sludge of 2 to 45,000 µg/L (Bennett, 1989; U.S. EPA, 1982). The same survey reported concentrations

1142 of BBP in digested sludge of not detected to 4,400 µg/L, demonstrating that digestion may reduce

- 1143 sludge concentrations. The survey also reported an average BBP concentration of  $809 \,\mu$ g/L in
- 1144 undigested combined sludge for 21 WWTPs that did not have measurable concentrations in the influent,
- 1145 which indicates that BBP can accumulate in sludge during the wastewater treatment process. An
- additional EPA report measured BBP concentrations in combined sludge of 0.52 to 210 mg/kg dw
- (<u>Howie, 1991; Naylor and Loehr, 1982</u>). Another study conducted in the U.S. reported a biosolids
  concentration of 0.07 mg/kg after anaerobic digestion for an activated sludge WWTP in Florida (<u>Howie,</u>
- 1149 1150

1991).

BBP has also been consistently monitored for and detected in sludge, biosolids, and biosolids-amended soils across the world. Four studies conducted in China reported BBP concentrations in sludge of 0.023 to 35 mg/kg dw, with a mean of 0.39 mg/kg dw, at 11 WWTPs (Cai et al., 2007a); below detection to 1.4 mg/kg dw, with a mean of 0.14 mg/kg dw, at 25 WWTPs (Meng et al., 2014); 0.0011 to 0.0149 mg/kg, with a mean of 0.0048 mg/kg and detection rate of 80.4 percent, at 46 WWTPs (Zhu et al., 2019); and below detection to 16.69 mg/kg at 3 WWTPs (Wu et al., 2019). Compost made from biosolids in China had BBP concentrations of 0.045 to 0.36 mg/kg dw (Cai et al., 2007b).

1158

1159 Studies conducted in Europe found concentrations of BBP of 7 mg/kg in sludge prior to anaerobic

1160 digestion (Palm et al., 1989); below detection in 15 sludge samples (Fromme et al., 2002); below detection in anaerobically digested and dewatered biosolids (Marttinen et al., 2003);  $2.01 \times 10^{-1}$  mg/kg in 1161 1162 anaerobically digested biosolids (Gibson et al., 2005); and approximately 0.14 mg/kg dw in biosolids 1163 (Tran et al., 2015). Two studies evaluated the accumulation of BBP in soil following land application of biosolids. One found that BBP was not accumulating in large amounts in the soil receiving the biosolids 1164 1165 (Tran et al., 2015). The other found BBP concentrations of 0.06, 0.01, and 29  $\mu$ g/kg following low, 1166 normal, and higher loading rates of biosolids, while unamended soils had concentrations ranging from  $6 \times 10^{-5}$  to  $3.8 \times 10^{-4}$  mg/kg (Vikelsøe et al., 2002). 1167

1168

1169 Additionally, two studies in Australia found BBP concentrations in sludge ranging from below detection to  $5.87 \times 10^{-2}$  mg/kg for three activated sludge WWTPs (Tan et al., 2008; Tan et al., 2007b). The same 1170 study also found BBP concentrations of  $2.4 \times 10^{-3}$  to  $3.9 \times 10^{-3}$  mg/kg in two soils amended with 1171 biosolids. Other studies from across the world found BBP concentrations in sludge of 1 to 4 mg/kg 1172 (Gani and Kazmi, 2016);  $2.6 \times 10^{-2}$  to  $1.3 \times 10^{-1}$ , with a mean of  $7.6 \times 10^{-2}$  mg/kg, from three WWTPs 1173 (<u>Salaudeen et al., 2018a</u>);  $6.3 \times 10^{-2}$  to  $1.5 \times 10^{-1}$  mg/kg dw,  $6.6 \times 10^{-2}$  to  $1.1 \times 10^{-1}$  mg/kg dw, and below 1174 detection to 1.9×10<sup>6</sup> mg/kg at municipal WWTPs, mixed waste WWTPs, and industrial WWTPs, 1175 1176 respectively (Lee et al., 2019).

1177

1181

1178 Overall, the data indicate that BBP is likely to be present in biosolids but that it is unlikely to be 1179 persistent or mobile in soils after land application of biosolids given its K<sub>OC</sub>, water solubility, and

1180 biodegradation half-life in soil.

### 6.3.3 Landfills

1182 For the purpose of this assessment, landfills will be considered to be divided into two zones: an "upper-1183 landfill" zone, with normal environmental temperatures and pressures, where biotic processes are the 1184 predominant route of degradation for BBP, and a "lower-landfill" zone where elevated temperatures and pressures exist, and abiotic degradation is the predominant route of degradation for BBP. In the upper-1185 1186 landfill zone where oxygen may still be present in the subsurface, conditions may still be favorable for 1187 aerobic biodegradation. However, photolysis and hydrolysis are not considered to be significant sources 1188 of degradation in this zone. In the lower-landfill zone, conditions are assumed to be anoxic, and 1189 temperatures present in this zone are likely to inhibit biotic degradation of BBP. Temperatures in lower

landfills may be as high as 70 °C. At temperatures at and above 60 °C, biotic processes are significantly
inhibited, and are likely to be completely irrelevant at 70 °C (Huang et al., 2013).

1192

1193 BBP is deposited in landfills continually and in high amounts from the disposal of consumer products 1194 containing BBP. However, due to its low water solubility (2.69 mg/L), concentrations of BBP in landfill 1195 leachate are expected to be low. BBP is likely to be persistent in landfills due to the expected low rates 1196 of anaerobic biodegradation in lower-landfills, whereas some aerobic biodegradation may occur in 1197 upper-landfills. BBP is expected to form monophthalate ester products in landfill environments: 1198 Eilertsson et al. (1996) assessed the biodegradation of BBP employing anaerobic microbes originating 1199 from methanogenic landfill conditions in a laboratory reactor. In an incubation with nutrient media, the 1200 cultivated landfill methanogens vielded 11 percent of the theoretical methane production of BBP with 1201 less than 30 percent of the original BBP dose (50 mg-C/L) recoverable by day 278. Phthalate, 1202 monobenzyl phthalate,  $CH_4$  and  $CO_2$  reported as degradation products. However, the sterilization of the 1203 abiotic control failed in this study, therefore reported losses may not be entirely attributable to microbial 1204 degradation. As biodegradation rates may be suppressed in higher-temperature layers of landfills, it has 1205 been suggested that hydrolysis may be the main route of abiotic degradation of phthalate esters (Huang 1206 et al., 2013). Hydrolysis of BBP in landfill environments may be accelerated in more acidic zones (see 1207 Section 4.2 for more information on BBP hydrolysis).

1208

Due to the expected persistence of BBP in landfills, it may dissolve into leachate in small amounts as mentioned above. However, given its tendency to adsorb to organic phases in soils and solid media, migration to groundwater from leachate is not expected to be an important transport pathway. This conclusion is generally supported by landfill leachate studies, as summarized below.

1213 1214 Limited evidence for BBP leaching from landfill media is in part due to low detection frequencies 1215 obtained for BBP. Concentrations of less than 5 (LOD) to 8.1 µg/L were measured in leachates from a 1216 municipal landfill in Gryta, Västerås, Sweden (Öman and Hynning, 1993). Similarly, low detection 1217 frequencies for BBP were reported in a Japanese monitoring study of five leachate treatment facilities 1218 each employing different landfill and leachate treatment processes, and each having operated for various 1219 amounts of time (Asakura et al., 2007). The authors reported detection frequencies ranging from 0 1220 percent to 33 percent, where the five influent leachates had a detection frequency of 18 percent, and 1221 median and maximum concentrations of 3.3 and 5.7  $\mu$ g/L, respectively (<u>Asakura et al., 2007</u>). 1222

1223 Liu et al. (2010) measured phthalate esters in samples taken around an operational landfill in Wuhan 1224 city, China. BBP was not detected in any samples from the landfill leachate (n = 5), adjacent surface 1225 water (n = 4), and groundwater (n = 8) near the site (LOD range 22 to 341 ng/L). To compare, DEHP 1226 saw 60, 100 and 50 percent detection frequencies in these media. BBP was detected in three topsoil 1227 samples (topsoil concentrations ranging from ND to  $61.4 \,\mu g/kg$ ) and one overbarden (top layer) sample 1228 at 180.9 µg/kg. The authors note that the reported concentrations were blank and recovery-corrected, 1229 however, no additional quality control data was explicitly provided (Liu et al., 2010). In the U.S., BBP 1230 was not detected (LOD 0.3 mg/kg) in a survey of construction and demolition waste in Florida, whereas 1231 DBP was measured ranging from 0.4 to 7.8 mg/kg (Jang and Townsend, 2001). 1232

- 1232 The low detection frequencies in leachates are supported by a report studying the leaching behavior of
  - 1234 two polyvinyl butyral (PVB) products in various leaching media using a method proposed by U.S. EPA
  - 1235 for Toxicity Characteristic Leaching Procedure (TCLP) (Monsanto, 1986b). In this controlled laboratory
  - 1236 leaching potential study, <u>Monsanto (1986b)</u> studied the leaching BBP behavior of two types of Saflex®
  - 1237 PVB (identified as TG and SR) using a method proposed by U.S. EPA for Toxicity Characteristic
  - 1238 Leaching Procedure (TCLP) with four leaching media: sodium acetate (NaOAc), acetic acid (HOAc),
hydrochloric acid (HCl), and sodium hydroxide (NaOH). BBP was not detected in any of the leachates of the TG Saflex® leaching tests. However, BBP was detected at concentrations of 0.28, 0.34 and 0.28 mg/L when leaching the SR Saflex® with HOAc, HCL and NaOAc, respectively. BBP concentration in a characteristic receptor well 500 ft away was then modeled to be 0.2 mg/L using a vertical-horizontal spread model and the TCLP results as the starting concentration (<u>Monsanto, 1986b</u>). Given the physical and chemical properties of BBP along with available monitoring data, BBP is expected to remain largely adsorbed to solids in landfills, with minimal transport in leachates.

# 6.3.4 Groundwater

There are several potential sources of BBP in groundwater, including from infiltration of wastewater effluents and to a lesser degree, landfill leachates (discussed in Sections 7.2 and 6.3.3, respectively). Furthermore, in environments where BBP is found in surface water, it may enter groundwater through surface water/groundwater interactions, especially in areas with groundwater-fed surface waters. Diffuse sources include stormwater runoff and runoff from biosolids applied to agricultural land, though these are expected to be minimal due to the physical and chemical characteristics—namely solubility and hydrophobicity—of BBP.

1254

1246

Given the strong affinity of BBP to adsorb to organic matter present in soils (log  $K_{OC} = 3.38-4.23$  L/kg) (Russell and Mcduffie, 1986; Monsanto, 1983b), BBP is expected to have low mobility in soil and therefore a low tendency to migrate to groundwater. Furthermore, due to the low solubility of BBP (2.69 mg/L), high dissolved concentrations of DBP in groundwater are unlikely. In instances where BBP could reasonably be expected to be present in groundwater environments (potentially, proximal to landfills or agricultural land with a history of land applied biosolids), limited persistence is expected based on rates of biodegradation of BBP in aerobic and anaerobic environments (see Section 4.1).

# 12621263 7 PERSISTENCE POTENTIAL OF BBP

1264 BBP is not expected to be persistent in the environment, as the overall environmental half-life was estimated to be approximately 8.9 days using the Level III Fugacity model in EPI Suite<sup>TM</sup> (U.S. EPA, 1265 2012). Biodegradation half-lives on the order of days to months are expected in most aquatic, soil, and 1266 1267 sediment environments (Section 4.1). With an expected indirect photolysis half-life of less than one day, 1268 BBP is unlikely to be persistent in the atmosphere (Section 4.3). BBP is predicted to hydrolyze slowly at 1269 ambient temperature but is not expected to persist in aquatic media as it undergoes rapid aerobic 1270 biodegradation (Section 4.2). Data also show that BBP is not likely to bioaccumulate in aquatic or 1271 terrestrial organisms (Section 8).

# 1272 **7.1 Destruction and Removal Efficiency**

1273 Destruction and Removal Efficiency (DRE) is a percentage that represents the mass of a pollutant 1274 removed or destroyed in a thermal incinerator relative to the mass that entered the system. BBP is 1275 classified as a hazardous substance and EPA requires that hazardous waste incineration systems destroy 1276 and remove at least 99.99 percent of each harmful chemical in the waste, including treated hazardous 1277 waste (46 FR 7684) (Federal Register, 1981). EPA extracted one study reporting on the DRE of BBP, 1278 which reported values of 99.92 to greater than 99.9996 percent for three incinerators using both aqueous 1279 and organic liquid wastes (Midwest Research Institute, 1984). Therefore, it is expected that BBP will be 1280 fully destroyed during most incineration processes.

# 1281**7.2 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

1284 secondary treatments. During the primary treatment, screens, grit chambers, and settling tanks are used 1285 to remove solids from wastewater. After undergoing primary treatment, the wastewater undergoes a

1286 secondary treatment. Secondary treatment processes can remove up to 90 percent of the organic matter

1287 in wastewater using biological treatment processes such as trickling filters or activated sludge.

1288 Sometimes an additional stage of treatment such as tertiary treatment is utilized to further clean water

1289 for additional protection using advanced treatment techniques (e.g., ozonation, chlorination, disinfection).

1290 1291

1292 The available data sources report overall removal efficiencies of BBP in conventional activated sludge 1293 WWTPs of 41 to 93 percent (Table 7-1). The water solubility (2.69 mg/L) and log  $K_{OC}$  (4.86) of BBP 1294 suggest partial removal via sorption to sludge in WWTPs. Biodegradation studies also suggest that both 1295 aerobic and anerobic biodegradation will also be important removal mechanisms during wastewater 1296 treatment (Section 4.1).

1297

1298 Studies evaluating overall removal efficiencies in WWTPs with activated sludge secondary treatment 1299 reported values of 43 to 87 percent at three WWTPs in South Africa (Salaudeen et al., 2018a, b); 66 1300 percent at a WWTP in Denmark (Fauser et al., 2003); 72 to 90 percent for two WWTPs in Hong Kong (Wu et al., 2017); 73.91 to 74.86 percent for WWTPs in China (Wu et al., 2019); greater than 80 percent 1301 1302 on average for five POTWs in the U.S. and 0 to 20 percent removal for one WWTP in the U.S. 1303 (Oppenheimer et al., 2007; Stephenson, 2007); 96 percent for a WWTP in France; and 50 percent and 1304 greater than 90 percent for a conventional activated sludge process and sequencing batch reactor in India, respectively (Gani and Kazmi, 2016). Salaudeen et al. (2018b) also reported removal efficiencies 1305 1306 of 89 percent and 88 percent for WWTPs using an oxidation pond and trickling filter, respectively. Two 1307 studies also reported lower removal efficiencies of 28 percent for a chemical enhanced primary 1308 treatment WWTP in Hong Kong with no secondary treatment (Wu et al., 2017) and 41 percent for a 1309 WWTP in India using an up flow anaerobic sludge blanket reactor followed by a finishing pond; 1310 however, since these treatment processes are not common in the U.S., they are not considered in this 1311 analysis. Additionally, one study conducted in China using three activated sludge WWTPs found no 1312 removal for one plant and a 40 to 230 percent increase for the other two (Gao et al., 2014). Across all 1313 available studies, both sorption to sludge and biodegradation were reported as primary removal 1314 mechanisms. 1315

1316 Additionally, the EPA 40 POTW study reported secondary treatment removal efficiencies for WWTPs 1317 across the U.S. with a variety of treatment processes, including activated sludge, trickling filters, and 1318 aerated lagoons. The study found that secondary treatment removal efficiency was greater than 50 1319 percent for greater than 99 percent of the POTWs and greater than 90 percent for 40 percent of the 1320 POTWs for the 35 WWTPs with BBP influent concentrations greater than 0 (U.S. EPA, 1982). Percent 1321 removals of BBP of 62 to 93 percent were calculated for plants with average influent concentrations 1322 greater than three times the most frequent detection limit of each WWTP (U.S. EPA, 1982).

1323

1324 It has also been shown that anaerobic sludge digestion can potentially reduce BBP concentrations in 1325 biosolids, with one study reporting a 74.3 to 76.4 percent decrease in BBP solids concentrations 1326 following anaerobic digestion for two WWTPs (Armstrong et al., 2018). The same study also reported 1327 that for two WWTPs there was either no change or an increase in BBP concentrations in solids 1328 following anaerobic digestion (Armstrong et al., 2018). These results indicate that anaerobic digestion 1329 may be an effective treatment process, but the efficiency will depend on the specific operating

1330 conditions of the digester and microbial community present.

1331

Modeling using STPWIN<sup>™</sup> in EPI Suite<sup>™</sup> showed that 99.86 percent of BBP will be removed during 1332

1333 conventional wastewater treatment when using biodegradation half-lives predicted by the BIOWIN<sup>TM</sup> model in EPI Suite<sup>TM</sup> (U.S. EPA, 2017). The half-lives predicted by the BIOWIN<sup>TM</sup> model are 1334 comparable to but shorter than the average half-lives in water identified in Section 4.1; therefore, the 1335 presented STPWIN<sup>TM</sup> results are likely representative of a high biodegradation scenario. The model also 1336 predicted that 81.54 percent of BBP would be removed by biodegradation and 18.31 percent would be 1337 1338 sorbed to sludge. Additional fugacity modeling of a conventional activated sludge WWTP in Australia 1339 that included biodegradation predicted an overall removal rate of 47 percent, with biodegradation being 1340 the major removal mechanism (Tan et al., 2007a). Overall, the available information suggests that both biodegradation and sorption to solids will be important removal mechanisms during aerobic wastewater 1341 1342 treatment. Additionally, air stripping is not expected to be a significant wastewater removal process 1343 based on the vapor pressure and HLC of BBP. In general, based on the available measured and predicted 1344 information, WWTPs are generally expected to remove between 40 to 90 percent of BBP present in wastewater.

- 1345
- 1346

Property	Removal Efficiency	<b>Reference</b> (s)	Data Quality Rating
	42.53–87.23%; activated sludge	Salaudeen et al. (2018a)	High
	66%; activated sludge	Fauser et al. (2003)	High
	50–90%; activated sludge	Gani and Kazmi (2016)	High
	0% for 1 WWTP, 40-230% increase for 2 WWTPs; activated sludge	<u>Gao et al. (2014)</u>	High
Removal (WWTP)	62–93%; activated sludge, tickling filters, aerated lagoons	<u>U.S. EPA (1982)</u>	High
	>80% for 6 WWTPs, 0–20% for 1 WWTP; activated sludge	Oppenheimer et al. (2007), Stephenson (2007)	High
	96%; activated sludge	<u>Tran et al. (2014)</u>	High
	73.91–74.86%; activated sludge	<u>Wu et al. (2019)</u>	High
	72–90%; activated sludge	<u>Wu et al. (2017)</u>	High
	76–89%; activated sludge,	Salaudeen et al. (2018b)	High

Table 7-1. Summary of WWTP Removal Information for BBP 1347

1348

#### 7.3 Removal in Drinking Water Treatment 1349

Drinking water in the United States typically comes from surface water (*i.e.*, lakes, rivers, reservoirs) 1350 1351 and groundwater. The source water then flows to a treatment plant where it undergoes a series of water 1352 treatment steps before being dispersed to homes and communities. In the U.S., public water systems 1353 often use conventional treatment processes that include coagulation, flocculation, sedimentation, 1354 filtration, and disinfection, as required by law.

1355

1356 EPA did not identify any studies quantifying the removal of BBP in water treatment plants. EPA previously determined that the phthalates DBP and DIBP will be partially removed in conventional 1357

water treatment plants (U.S. EPA, 2024c, d). Given the similarity in structure and physical and chemical 1358

properties of BBP to DIBP and DBP, EPA expects BBP to be partially removed in water treatmentplants.

# 1362 8 BIOACCUMULATION OF BBP

The presence of BBP in several marine aquatic species in North America suggests that it may be
bioavailable in aquatic environments (Mackintosh et al., 2004); however, a measured log K<sub>OW</sub> of 4.34
suggests that BBP is not expected to have a high bioaccumulation potential. Further, an EPI Suite<sup>TM</sup>
predicted bioaccumulation factor (BAF) value of 40.1 L/kg wet weight suggests limited
bioaccumulation potential. EPA also identified nine high-quality data sources reporting the aquatic
bioconcentration, aquatic bioaccumulation, aquatic food web magnification, and terrestrial
bioconcentration of BBP (Table 8-1).

1370

1361

1371 EPA identified three studies measuring the bioconcentration factor (BCF) of BBP in bluegill sunfish. 1372 BCF values were quantified in two ways: 1) measurement of radio-labeled carbon concentrations in fish 1373 and water; and 2) measurement of direct concentrations of BBP in fish and water. The whole fish BCF value calculated using direct measurements of BBP was 12.4 (Carr et al., 1997), while whole fish BCF 1374 1375 values calculated using radio-labeled carbon were much higher at 187.65 to 663 (Carr et al., 1997; 1376 Monsanto, 1983a; Barrows et al., 1980). BCF values calculated using radio-labeled carbon can be artificially greater because concentrations in the fish will include metabolites and degradation products 1377 1378 of BBP, which may be more bioavailable than the parent compound. BCF values calculated using direct

measurement of BBP are more reflective of the bioconcentration potential of BBP; therefore, for this

- analysis, EPA relied on the BCF value of 12.4 from the study using direct measurements of intact BBPto assess the bioconcentration potential of BBP.
- 1382

1379

1383 EPA identified one study that reported total water concentration (dissolved + particulate) BAF values of 1384 204,000 L/kg-lipid for staghorn sculpin (Leptocottus armatus; a forage fish) and 11,800 L/kg-lipid for 1385 spiny dogfish (Squalus Acanthias; a flatfish) collected from False Creek, British Columbia (Gobas et al., 1386 2003). Adjusting for 5.0 percent lipid content for the staghorn sculpin, and 15 percent lipid content for the dogfish, the non-lipid normalized BAF values from this study are 10,200 L/kg and 1,770 L/kg, 1387 1388 respectively (Gobas et al., 2003). The study further reported lipid equivalent BAF values greater than 1389 100,000 L/kg-lipid for green algae (Enteromorpha intestinalis), plankton, geoduck clams (Panopea 1390 abrupta), clams, striped seaperch (Embiotoca lateralis), pile perch (Rhacochilus vacca), and surf scoters 1391 (Melanitta perspicillata). These BAF values indicate that BBP has bioaccumulation potential among the 1392 monitored species in False Creek and suggest that diet may be an appreciable route of exposure for 1393 aquatic organisms, as BAF values account for both respiration and dietary exposure routes. However, 1394 EPA was unable to confirm key experimental details required to assess the study quality, such as sample 1395 sizes, and quality control and quality assurance measures associated with both sampling and analytical 1396 methods of the study. As a result, EPA only has moderate overall confidence in representativeness of 1397 these reported BAF values.

- 1398
- 1399 One study measured a trophic magnification factor (TMF) of 0.77 in a marine environment, which 1400 indicates that biomagnification up an aquatic food chain is not likely (Anscher et al., 2006).
- Additionally, two studies reported biota-sediment accumulation factor (BSAF) values of 2 to 20 for five
- 1401 Additionary, two studies reported blota-sediment accumulation factor (BSAF) values of 2 to 20 for five 1402 species of fish from rivers in Taiwan (Huang et al., 2008) and 2.8 to 4.3 for three species of fish from
- the Orge river in France (<u>Teil et al., 2012</u>) (Table 8-1). In general, the measured data suggest that BBP
- 1404 will have a low biomagnification and trophic magnification potential in aquatic organisms based on the
- 1405 measured BCF, TMF, and BSAF values; however, the measured BAF values indicate that
- 1406 bioaccumulation in fish may be possible in certain scenarios and may tend to accumulate more readily in
- 1407 lower-trophic level species and species that associate more with benthic sediments. Because of limited

- 1408 empirical BAF data that generally disagree with the modeled BCFBAF<sup>TM</sup> BAF estimate and empirical
  1409 BCF data available for BBP, EPA has slight confidence that BBP will not bioaccumulate in aquatic
  1410 organisms.
- 1411
- 1412 EPA identified two studies that report BAF values for BBP in terrestrial environments. One study
- 1413 reported values of 6.79 to 35.75 for wheat and 1.41 to 2.90 for maize (Li et al., 2018). The other study
- 1414 measuring concentrations of BBP in vegetables did not detect BBP in any of the vegetables sampled (n
- 1415 = 16), which indicates no terrestrial bioaccumulation potential (<u>Li et al., 2016a</u>). Overall, the measured
- 1416 data suggest that BBP will have a low bioaccumulation and biomagnification potential in terrestrial
- 1417 organisms.
- 1418

## 1419 **Table 8-1. Summary of Bioaccumulation Information for BBP**

Endpoint	Value	Organism	Reference	Overall Quality Ranking
	Whole fish: 12.4; viscera: 19.1; fillet: 1.1 (intact BBP)	Bluegill sunfish ( <i>Lepomis macrochirus</i> )	<u>Carr et al. (1997)</u>	High
	Whole fish: 225; viscera- 387: fillet: 25.5 (radio-labeled carbon)			
Aquatic BCF	Whole fish: 187.65 (radio-labeled carbon)	Bluegill sunfish ( <i>Lepomis macrochirus</i> )	Monsanto (1983a)	High
	Whole fish: 663 (radio-labeled carbon)	Bluegill sunfish ( <i>Lepomis macrochirus</i> )	Barrows et al. (1980)	High
A quatia PAE	Total water concentration: 11,800 L/kg-lipid; observed lipid equivalent: 11,800 L/kg-lipid	Dogfish (Squalus Acanthias)	Gobas et al. (2003)	Medium
Aquaic BAF	Total water concentration- 72,700 L/kg lipid: observed lipid equivalent- 204,000 L/kg lipid	Sculpin ( <i>Leptocottus</i> armatus)		
Aquatic BSAF	2–20	Blackhead seabream ( <i>Acanthopagrus schlegeli</i> , <i>Liza subviridis</i> - B), Nile tilapia ( <i>Oreochromis</i> <i>miloticus niloticus</i> - c), and	<u>Huang et al. (2008)</u>	High

Endpoint	Value	Organism	Reference	Overall Quality Ranking
		Taiwan Torrent Carp (Acrossocheilus paradoxus)		
	2.8-4.3	Perch ( <i>Perca fluviatilis</i> ), roach ( <i>Rutilus rutilus</i> ), and chub ( <i>Leuciscus cephalus</i> )	<u>Teil et al. (2012)</u>	High
Aquatic TMF	0.77	Marine food chain, including plankton, microalgae, blue mussels ( <i>Mytilus edulis</i> ), geoduck clams ( <i>Panopea</i> <i>abrupta</i> ), striped seaperch ( <i>Embiotoca lateralis</i> ), and spiny dogfish ( <i>Squalus</i> <i>acanthias</i> )	<u>Mackintosh et al.</u> (2004)	High
	Wheat: 6.79–35.75; maize: 1.41–2.90	Winter wheat ( <i>Triticum</i> <i>aestivum</i> ), and summer maize ( <i>Zea mays</i> )	<u>Li et al. (2018)</u>	High
Terrestrial BAF	Not detected in vegetables	Vegetables collected from a greenhouse (n=16), including eggplant, bitter gourd, peppers, tomato, long podded cowpea, celery, onion	<u>Li et al. (2016a)</u>	High

1420 1421

# 1422 9 OVERALL FATE AND TRANSPORT OF BBP

1423 The inherent physical and chemical properties of BBP govern its environmental fate and transport. The 1424 magnitude of the partitioning coefficients identified for BBP (Table 5-2) suggest that BBP may exist in 1425 surface water, and sorbed to organic carbon fractions in soil, sediment, and air in the environment. With 1426 a HLC of  $7.61 \times 10^{-7}$  atm·m<sup>3</sup>/mol at 25 °C (<u>Elsevier, 2019</u>), BBP is not expected to be volatile from 1427 surface water. BBP is slightly soluble in water (2.69 mg/L (NLM, 2015)), and sorption to organics present in sediment and to suspended and dissolved solids present in water is expected to be a dominant 1428 1429 process given the range of identified log K<sub>oc</sub> values (Table 5-1). BBP's solubility and range of log K<sub>oc</sub> 1430 values (Table 5-1) suggests that BBP that occurs in soil is unlikely to exhibit mobility, also supported by 1431 fugacity modeling (Section 5).

1432

BBP in surface water is subject to two primary competing processes: biodegradation and adsorption to

1434 organic matter in suspended solids and sediments. BBP in the freely dissolved phase is expected to show

1435 low persistence, with rapid biodegradation under aerobic conditions (Table 4-1). The fraction of BBP

adsorbed to particulates increases with water salinity due to a salting out effect, as indicated by greater
 log K<sub>OC</sub> values measured in saltwater as compared to those measured with freshwater. Monitoring data

1437 log K<sub>OC</sub> values measured in sativater as compared to mose measured with reshwater. Monitoring data 1438 in the U.S. generally show low detection frequencies in surface water. Sampling of U.S. surface water

sediments yielded a wide range of concentrations, however BBP was generally found in lower

- 1440 concentrations than other phthalate esters and often with low detection frequencies. However,
- monitoring data have historically shown concentrations up to 16,000  $\mu$ g/kg in river sediments (<u>Papoulias</u> and Buckler, 1996).
- 1443

BBP has a vapor pressure of 8.25×10<sup>-6</sup> mmHg at 25 °C (NLM, 2015; Howard et al., 1985) indicating 1444 that BBP will preferentially adsorb to particulates in the atmosphere, with adsorbed fractions being 1445 1446 resistant to photolysis. This is consistent with the estimated octanol:air partition coefficient of 9.2 (U.S. 1447 EPA, 2017). BBP that occurs in the atmosphere will likely degrade via ·OH-mediated indirect photolysis 1448 with a half-life of 0.97 days (23.28 hours) based on an estimated  $\cdot$ OH reaction rate constant of  $1.10 \times 10^{-1}$ 1449 <sup>11</sup> cm<sup>3</sup>/molecule-second, and assuming a 12-hour day with  $1.5 \times 10^6 \cdot \text{OH/cm}^3$  (U.S. EPA, 2017). BBP is 1450 consistently detected at low concentrations in ambient air (Section 6.1.1); however, given its 1451 atmospheric half-life, BBP is not expected to be persistent in air or undergo long range transport. 1452

- BBP in indoor settings is expected to partition to airborne particles and dust. BBP in indoor air is also
  likely to have a longer half-life compared to ambient outdoor air due to limited direct and indirect
  photolysis. The available data suggest that plastic products containing are likely to be sources of BBP in
  indoor environments (Dodson et al., 2017; Abb et al., 2009).
- 1457

BBP arrives to landfills via the disposal of consumer products containing BBP. Limited information is
available on the biodegradation potential of BBP in landfill media. However, given the physical and
chemical properties of BBP along with available monitoring data and experimental leaching data, BBP
is expected to remain largely adsorbed to solids in landfills, with minimal transport in leachates.

1462

1463 Limited information is available on the removal of BBP during drinking water treatment; however, it is 1464 expected to behave similarly to other phthalate esters exhibiting partial removal. Based on BBP's 1465 aqueous solubility, slight tendency to volatilize, and strong tendency to adsorb to organic carbon, this 1466 chemical substance will readily partition to solids in wastewater treatment processes. Additionally, 1467 biodegradation may represent a significant proportion of BBP's removal rate, as BBP is readily biodegradable under aqueous, aerobic conditions (Table 4-1). Available information on overall WWTP 1468 removal rates indicate a wide range of efficiencies, generally falling between 40 to 90 percent (Table 1469 1470 7-1), with biodegradation and adsorption as the dominant mechanisms. Overall, the data indicate that 1471 BBP is likely to be present in biosolids but that it is unlikely to be persistent or mobile in soils after land 1472 application of biosolids given its K<sub>OC</sub>, water solubility, and biodegradation half-life in soil (Table 4-1). 1473

1474 10 WEIGHT OF THE SCIENTIFIC EVIDENCE AND CONCLUSIONS
 1475 ON THE FATE AND TRANSPORT OF BBP

# 1476 10.1 Strengths, Limitations, Assumptions, and Key Sources of Uncertainty 1477 for the Fate and Transport Assessment

Given the consistent results from numerous high-quality, empirical studies, there is a robust confidencethat BBP:

- will partition to organic carbon and particulate matter in air, with a measured vapor pressure of 8.25×10<sup>-6</sup> mmHg (NLM, 2015; Howard et al., 1985) and a log K<sub>OA</sub> of 9.2 (U.S. EPA, 2017) (Sections 5 and 6.1);
- will readily biodegrade in aerobic, aqueous environments including during wastewater treatment
   (Section 7.2) and in surface waters (Section 4.1). Biodegradation rates of BBP in water will

1485	depend on the microbial community, organic matter presence, and previous exposure/adaptation
1486	to BBP.
1487	• will readily biodegrade in aerobic surface sediments (Section 4.1), however fractions bound to
1488	sediment are expected to present longer persistence until release by a shift in equilibrium;
1489	• is expected to biodegrade under anaerobic conditions, however generally more slowly than under
1490	aerobic conditions. As with aerobic degradation anaerobic biodegradation rates of BBP are
1491	likely to depend on the microbial community organic matter presence and previous
1497	exposure/adaptation to BBP (Sections 4.1 and 6.2.2).
1/03	• will be removed in westewater treatment plants at 40 to 90 percent, with sorption to sludge and
1493	biodegradation both being significant removal mechanisms (Section 7.2):
1404	<ul> <li>presents low bioconcentration potential in fish: however, monophthelates (monobuty) and</li> </ul>
1495	• presents low bioconcentration potential in fish, nowever, monophilatates (monobuly) and
1490	monobenzyl phinalate) exhibited slightly elevated bioconcentration potential as compared to
1497	parent DDF (Section 8), will not high and will awhibit transis dilution in aquatic appairs (Section 8).
1498	• will not bioinaginity and will exhibit dopine dilution in aquatic species (Section 8);
1499	• is likely to be present in biosolids, though is unlikely to be persistent or mobile in soils after land
1500	application of biosolids given its $K_{OC}$ , water solubility, and biodegradation processes;
1501	• will not exhibit substantial mobility to groundwater from soil or landfill environments, and will
1502	tend to stay sorbed to solid organics in soil media and landfills; and
1503	• 1s likely to be found in household dust (Section 6.1.2).
1504	
1505	As a result of limited empirical studies identified, there is a moderate confidence that BBP:
1506	• will not exhibit persistence in air, and undergo indirect photodegradation by reacting with
1507	hydroxyl radicals in the atmosphere with a half-life of 1.13 to 1.15 days (Section 4.3);
1508	<ul> <li>will be removed in conventional drinking water treatment systems (Section 7.3);</li> </ul>
1509	• may show persistence in surface water, sediment, and soil proximal to continuous points of
1510	release, in cases where the release rate exceeds the rate of biodegradation (Sections 3.2, 5);
1511	• does not biodegrade in anaerobic environments (Section 5.2, 5.3);
1512	• will undergo aerobic and anaerobic biodegradation in soil and landfill media under conducive
1513	conditions (Sections 6.3.1 and 6.3.3, respectively);
1514	• is expected to have a low tendency to migrate to groundwater, however explicit groundwater fate
1515	studies are limited for BBP; and
1516	• will not undergo appreciable hydrolysis in aqueous systems, as biodegradation is expected to
1517	occur much more rapidly under most conditions (Sections 4.1 and 4.2); however, hydrolysis may
1518	be important in deep, acidic, thermophilic landfill environments (Section 6.3.3).
1519	
1520	As a result of no empirical studies identified, there is a slight confidence that BBP:
1521	• presents low bioaccumulation potential in aquatic species (Section 8).
1522	presente le la croate antannical potential in adante species (secure o).
1523	Findings that were found to have a robust weight of evidence supporting them had one or more high-
1524	quality studies that were largely in agreement with each other. Findings that were said to have a
1525	moderate weight of evidence were based on a mix of high and medium-quality studies that were largely
1526	in agreement, but varied in sample size and consistence of findings, or when both modeling and
1527	empirical information was used in support of the conclusion. Findings said to have a slight weight of
1500	avidance had limited and contracting ampirical avidance in support of the conclusion

1528 evidence had limited and contrasting empirical evidence in support of the conclusion.

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# 2057 APPENDICES

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2058
                  COMPLETE RESULTS FROM EPI Suite<sup>TM</sup> MODELING
     Appendix A
2059
2060
     CAS Number: 000085-68-7
2061
     SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c2
2062
     CHEM : Benzyl butyl phthalate
2063
     MOL FOR: C19 H20 O4
2064
     MOL WT : 312.37
2065
     ----- EPI SUMMARY (v4.11) -----
2066
2067
      Physical Property Inputs:
2068
      Log Kow (octanol-water):
                              4.73
2069
       Boiling Point (deg C) : 370.00
       Melting Point (deg C) : -35.00
2070
        Vapor Pressure (mm Hg) : 8.25E-006
2071
2072
        Water Solubility (mg/L): 2.69
2073
        Henry LC (atm-m3/mole) : 7.1E-007
2074
2075
     KOWWIN Program (v1.68) Results:
2076
     _____
2077
2078
                   Log Kow (version 1.69 estimate): 4.84
2079
2080
     Experimental Database Structure Match:
2081
     Name : BUTYL BENZYL PHTHALATE
2082
       CAS Num : 000085-68-7
2083
      Exp Log P: 4.73
2084
      Exp Ref : ELLINGTON, JT & FLOYD, TL (1996)
2085
2086
     SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c2
2087
     CHEM : Benzyl butyl phthalate
2088
     MOL FOR: C19 H20 O4
2089
     MOL WT : 312.37
2090

      TYPE
      NUM
      LOGKOW FRAGMENT DESCRIPTION
      | COEFF
      VALUE

2091
2092
     _____+
2093
     Fraq | 1 | -CH3 [aliphatic carbon]
                                                    | 0.5473 | 0.5473
     Frag | 4 | -CH2- [aliphatic carbon]
2094
                                                    | 0.4911 | 1.9644
     Frag | 12 | Aromatic Carbon
2095
                                                    | 0.2940 | 3.5280
2096
     Frag | 2 | -C(=0)0 [ester, aromatic attach] |-0.7121 | -1.4242
2097
     Const | | Equation Constant
                                                    | 0.2290
2098
     _____+
2099
                                                    Log Kow = 4.8445
2100
2101
2102
2103
     MPBPVP (v1.43) Program Results:
2104
     _____
2105
     Experimental Database Structure Match:
2106
      Name : BUTYL BENZYL PHTHALATE
2107
      CAS Num : 000085-68-7
2108
      Exp MP (deg C): -40.5
2109
      Exp BP (deq C): 370
2110
      Exp VP (mm Hq): 8.25E-06
             (Pa ): 1.10E-003
2111
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```
2112
          Exp VP (deg C): 25
2113
         Exp VP ref : HOWARD, PH ET AL. (1985)
2114
2115
        SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c2
2116
        CHEM : Benzyl butyl phthalate
2117
        MOL FOR: C19 H20 O4
2118
        MOL WT : 312.37
2119
        ----- SUMMARY MPBPWIN v1.44 -----
2120
2121
2122
        Boiling Point: 387.45 deg C (Adapted Stein and Brown Method)
2123
2124
       Melting Point: 50.75 deg C (Adapted Joback Method)
2125
        Melting Point: 112.57 deg C (Gold and Ogle Method)
2126
        Mean Melt Pt : 81.66 deg C (Joback; Gold, Ogle Methods)
2127
       Selected MP: 61.05 deg C (Weighted Value)
2128
2129
       Vapor Pressure Estimations (25 deg C):
2130
        (Using BP: 370.00 deg C (user entered))
2131
         (MP not used for liquids)
2132
          : 0.00207 Pa (Antoine Method)
VP: 4.4F-005 mm U
          VP: 1.55E-005 mm Hg (Antoine Method)
2133
2134
            VP: 4.4E-005 mm Hg (Modified Grain Method)
          : 0.00587 Pa (Modified Grain Met
VP: 8.88E-005 mm Hg (Mackay Method)
2135
            : 0.00587 Pa (Modified Grain Method)
2136
2137
           : 0.0118 Pa (Mackay Method)
2138 Selected VP: 4.4E-005 mm Hg (Modified Grain Method)
2139
                     : 0.00587 Pa (Modified Grain Method)
2140
2141
2142
2143
        _____
2144
      TYPE | NUM | BOIL DESCRIPTION | COEFF | VALUE

      2145
      Group | 1 | -CH3
      21.98
      21.98

      2146
      Group | 4 | -CH2-
      24.22
      96.88

      2147
      Group | 2 | -COO- (ester)
      78.85
      157.70

      2149
      Group | 9 | CH (aromatic)
      28.53
      256.77

      2150
      Group | 3 | -C (aromatic)
      30.76
      92.28

      2151
      Corr | 1 | Diester-type
      -35.00
      -35.00

2152
        * | | Equation Constant | | 198.18
RESULT-uncorr | BOILING POINT in deg Kelvin | 788.79
2154
2155
       RESULT- corr | BOILING POINT in deg Kelvin | 660.61
2156
          | BOILING POINT in deg C | 387.45
2157
        _____
2158
2159
        _____+
2160
        TYPE | NUM | MELT DESCRIPTION | COEFF | VALUE
2161
       _____+

      2161
      Group | 1 | -CH3
      -5.10 | -5.10

      2162
      Group | 4 | -CH2
      11.27 | 45.08

      2164
      Group | 2 | -COO- (ester)
      53.60 | 107.20

      2165
      Group | 9 | CH (aromatic)
      8.13 | 73.17

      2166
      Group | 3 | -C (aromatic)
      37.02 | 111.06

      2167
      Corr | 1 | Diester-type
      -130.00 | -130.00

2168
        * | | Equation Constant |
                                                     | 122.50
```

2169 2170 RESULT | MELTING POINT in deg Kelvin | 323.91 2171 MELTING POINT in deg C 50.75 2172 \_\_\_\_\_ 2173 2174 2175 2176 Water Sol from Kow (WSKOW v1.42) Results: 2177 \_\_\_\_\_\_ 2178 2179 Water Sol: 4.635 mg/L 2180 2181 Experimental Water Solubility Database Match: 2182 Name : BUTYL BENZYL PHTHALATE 2183 CAS Num : 000085-68-7 2184 Exp WSol : 2.69 mg/L (25 deg C) 2185 Exp Ref : HOWARD, PH ET AL. (1985) 2186 2187 SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c22188 CHEM : Benzyl butyl phthalate 2189 MOL FOR: C19 H20 O4 2190 MOL WT : 312.37 2191 ------ WSKOW v1.43 Results -----2192 Log Kow (estimated) : 4.84 2193 Log Kow (experimental): 4.73 2194 Cas No: 000085-68-7 2195 Name : BUTYL BENZYL PHTHALATE 2196 Refer : ELLINGTON, JT & FLOYD, TL (1996) 2197 Log Kow used by Water solubility estimates: 4.73 (user entered) 2198 2199 Equation Used to Make Water Sol estimate: 2200 Log S (mol/L) = 0.693-0.96 log Kow-0.0092(Tm-25)-0.00314 MW + Correction 2201 2202 Melting Pt (Tm) = -35.00 deg C (Use Tm = 25 for all liquids) 2203 2204 Correction(s): Value 2205 ----- -----2206 No Applicable Correction Factors 2207 2208 Log Water Solubility (in moles/L) : -4.829 2209 Water Solubility at 25 deg C (mg/L): 4.635 2210 2211 2212 2213 WATERNT Program (v1.01) Results: 2214 \_\_\_\_\_ 2215 2216 Water Sol (v1.01 est): 1.0791 mg/L 2217 2218 Experimental Water Solubility Database Match: 2219 Name : BUTYL BENZYL PHTHALATE 2220 CAS Num : 000085-68-7 2221 Exp WSol : 2.69 mg/L (25 deg C) 2222 Exp Ref : HOWARD, PH ET AL. (1985) 2223 2224 SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c2 2225 CHEM : Benzyl butyl phthalate

2226 MOL FOR: C19 H20 O4 2227 MOL WT : 312.37 2228 2229 TYPE | NUM | WATER SOLUBILITY FRAGMENT DESCRIPTION | COEFF | VALUE 2231 Frag | 1 | -CH3 [aliphatic carbon] |-0.3213 | -0.3213 2232Frag4-CH2-[aliphatic carbon]2233Frag9Aromatic Carbon (C-H type) |-0.5370 | -2.1481 

 2233
 Frag | 9 | Aromatic Carbon (C-H type)
 |-0.3359 | -3.0228

 2234
 Frag | 2 | -C(=0)0 [ester, aromatic attach]
 | 0.7006 | 1.4012

 2235
 Frag | 3 | Aromatic Carbon (C-substituent type)
 |-0.5400 | -1.6199

 2236
 Const | | Equation Constant
 | Equation Constant

 Const | | Equation Constant | 0.2492 2237 2238 Log Water Sol (moles/L) at 25 dec C = -5.46162239 Water Solubility (mg/L) at 25 dec C = 1.0791 2240 2241 2242 2243 ECOSAR Program (v1.11) Results: 2244 \_\_\_\_\_ 2245 ECOSAR Version 1.11 Results Page 2246 2247 SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c2 2248 CHEM : Benzyl butyl phthalate 2249 CAS Num: 2250 ChemID1: 2251 MOL FOR: C19 H20 O4 2252 MOL WT : 312.37 MOL W1 : 512.57Log Kow: 4.845(EPI Suite Kowwin v1.68 Estimate)Log Kow:(User Entered)Log Kow: 4.73(PhysProp DB exp value - for comparison only)Melt Pt: -35.00(deg C, User Entered for Wat Sol estimate)Melt Pt: -40.50(deg C, PhysProp DB exp value for Wat Sol est)Wat Sol: 4.635(mg/L, EPI Suite WSKowwin v1.43 Estimate)Wat Sol: 2.69(mg/L, PhysProp DB exp value) 2253 2254 2255 2256 2257 2258 2259 2260 2261 2262 2263 \_\_\_\_\_ 2264 Values used to Generate ECOSAR Profile 2265 \_\_\_\_\_ Log Kow: 4.845 (EPI Suite Kowwin v1.68 Estimate) Wat Sol: 2.69 (mg/L, User Entered) 2266 2267 2268 2269 2270 2271 \_\_\_\_\_ 2272 ECOSAR v1.11 Class-specific Estimations 2273 \_\_\_\_\_ 2274 Esters 2275 Predicted 2276 Organism Duration End Pt mg/L (ppm) ECOSAR Class 2277 \_\_\_\_\_ : Fish 96-hr LC50 0.911 : Daphnid 48-hr LC50 1.397 : Green Algae 96-hr EC50 0.379 2278 Esters 2279 Esters 2280 Esters 2281 Esters ChV : Fish 0.038 2282 Esters : Daphnid ChV 0.421

Estors	: Green Algae	06-br	ChV	0.245
Esters	: Mvsid	96-hr	LC50	0.282
Esters	: Fish (SW)		ChV	0.279
Esters	: Mysid (SW)		ChV	0.063
Esters	: Earthworm	14-day	LC50	492.947
======================================	====== ===============================	=== ==================================	= ===== LC50	======== 0.716
(Baseline Toxicity)	: Daphnid	48-hr	LC50	0.528
	: Green Algae	96-hr	EC50	1.166
	: Fish		ChV	0.095
	: Green Algae		ChV	0.548
measure this water solubil are reported.	predicted effect. If the ity by 10X, typically no	e effects at	al exceeds saturatio	s the on (NES)
Class Specific LogKow	Cut-Offs			
endnoints				
Esters:  Maximum LogKow: 5.0 (	Fish 96-hr LC50; Daphnic	l LC50, Mysic	ł LC50)	
Esters:  Maximum LogKow: 5.0 ( Maximum LogKow: 6.0 ( Maximum LogKow: 6.4 ( Maximum LogKow: 8.0 (	Fish 96-hr LC50; Daphnic Earthworm LC50) Green Algae EC50) ChV)	ł LC50, Mysic	4 LC50)	
Esters:  Maximum LogKow: 5.0 ( Maximum LogKow: 6.0 ( Maximum LogKow: 6.4 ( Maximum LogKow: 8.0 ( Baseline Toxicity SAR	Fish 96-hr LC50; Daphnic Earthworm LC50) Green Algae EC50) ChV) Limitations:	l LC50, Mysic	ł LC50)	
Esters: Maximum LogKow: 5.0 ( Maximum LogKow: 6.0 ( Maximum LogKow: 6.4 ( Maximum LogKow: 8.0 ( Baseline Toxicity SAR Maximum LogKow: 5.0 ( Maximum LogKow: 5.0 ( Maximum LogKow: 6.4 ( Maximum LogKow: 8.0 (	Fish 96-hr LC50; Daphnic Earthworm LC50) Green Algae EC50) ChV) Limitations:  Fish 96-hr LC50; Daphnic Green Algae EC50) ChV)	A LC50, Mysic A LC50)	ł LC50)	
Esters: Maximum LogKow: 5.0 ( Maximum LogKow: 6.0 ( Maximum LogKow: 6.4 ( Maximum LogKow: 8.0 ( Baseline Toxicity SAR Maximum LogKow: 5.0 ( Maximum LogKow: 5.0 ( Maximum LogKow: 6.4 ( Maximum LogKow: 8.0 (	Fish 96-hr LC50; Daphnic Earthworm LC50) Green Algae EC50) ChV) Limitations:  Fish 96-hr LC50; Daphnic Green Algae EC50) ChV)	4 LC50, Mysic	4 LC50)	
Esters:  Maximum LogKow: 5.0 ( Maximum LogKow: 6.0 ( Maximum LogKow: 6.4 ( Maximum LogKow: 8.0 ( Baseline Toxicity SAR  Maximum LogKow: 5.0 ( Maximum LogKow: 5.0 ( Maximum LogKow: 8.0 ( HENRYWIN (v3.20) Prog	Fish 96-hr LC50; Daphnic Earthworm LC50) Green Algae EC50) ChV) Limitations:  Fish 96-hr LC50; Daphnic Green Algae EC50) ChV) ram Results:	4 LC50, Mysic	4 LC50)	
Esters:  Maximum LogKow: 5.0 ( Maximum LogKow: 6.4 ( Maximum LogKow: 6.4 ( Maximum LogKow: 8.0 ( Baseline Toxicity SAR  Maximum LogKow: 5.0 ( Maximum LogKow: 5.0 ( Maximum LogKow: 6.4 ( Maximum LogKow: 8.0 ( HENRYWIN (v3.20) Prog  Bond Est : 4. Group Est: 2.	Fish 96-hr LC50; Daphnic Earthworm LC50) Green Algae EC50) ChV) Limitations:  Fish 96-hr LC50; Daphnic Green Algae EC50) ChV) ram Results: ======= 22E-008 atm-m3/mole (4. 13E-009 atm-m3/mole (2.	4 LC50, Mysic 4 LC50) 28E-003 Pa-m 16E-004 Pa-m	13/mole)	
Esters:  Maximum LogKow: 5.0 ( Maximum LogKow: 6.0 ( Maximum LogKow: 6.4 ( Maximum LogKow: 8.0 ( Baseline Toxicity SAR  Maximum LogKow: 5.0 ( Maximum LogKow: 5.0 ( Maximum LogKow: 5.0 ( Maximum LogKow: 8.0 ( HENRYWIN (v3.20) Prog Bond Est : 4. Group Est: 2. SMILES : O=C(OCc(cccc CHEM : Benzyl butyl MOL FOR: C19 H20 O4	<pre>Fish 96-hr LC50; Daphnic Earthworm LC50) Green Algae EC50) ChV) Limitations:  Fish 96-hr LC50; Daphnic Green Algae EC50) ChV) ram Results: ======= 22E-008 atm-m3/mole (4. 13E-009 atm-m3/mole (2. 1)c1)c(c(ccc2)C(=0)OCCCC phthalate</pre>	A LC50, Mysic A LC50) 28E-003 Pa-m 16E-004 Pa-m 2)c2	13/mole)	

CAS Num Exp HLC Temper Exp Ref	<pre>: BUTYL BENZYL PHTHALATE : 000085-68-7 : 1.26E-06 atm-m3/mole (0.128 Pa-m3/mole) : 25 deg C : VP/WSOL</pre>			
CLASS	-+BOND CONTRIBUTION DESCRIPTION	++   COMMENT	V	ALUE
HYDROGEN HYDROGEN FRAGMENT FRAGMENT FRAGMENT FRAGMENT FRAGMENT	<pre>1 11 Hydrogen to Carbon (aliphatic) Bonds 9 Hydrogen to Carbon (aromatic) Bonds 3 C-C 1 1 C-Car 2 C-O 1 12 Car-Car 2 Car-Car 2 Car-CO 2 C0-0</pre>		-1 -1 0 2 3 2 C	
RESULT	BOND ESTIMATION METHOD for LWAPC VALUE	++   TOTAL	5	5.763
HENRYS LA	-+N CONSTANT at 25 deg C = 4.22E-008 atm-m3/mole = 1.73E-006 unitless = 4.28E-003 Pa-m3/mole	+		
 	GROUP CONTRIBUTION DESCRIPTION	COMMENI	.	VAI
	1 CH2 (Car)(O) 1 CH3 (X) 2 CH2 (C)(C) 1 CH2 (C)(O) 9 Car-H (Car)(Car) 1 Car (C)(Car)(Car) 2 Car (Car)(Car)(CO) 2 CO (O)(Car) 2 O (C)(CO)	ESTIMATE           	;               	0.0 -0.6 -0.3 -0.1 0.9 -1.6 9.1
RESULT	GROUP ESTIMATION METHOD for LOG GAMMA VALUE	TOTAL		7.(
HENRYS LA	<pre>N CONSTANT at 25 deg C = 2.13E-009 atm-m3/mole = 8.71E-008 unitless = 2.16E-004 Pa-m3/mole</pre>	+	+	

2397 2398 Log Koa: 9.267 2399 2400 SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c22401 CHEM : Benzyl butyl phthalate 2402 MOL FOR: C19 H20 O4 2403 MOL WT : 312.37 2404 ----- KOAWIN v1.10 Results -----2405 2406 Log Koa (octanol/air) estimate: 9.267 2407 Koa (octanol/air) estimate: 1.85e+009 2408 Using: 2409 Log Kow: 4.73 (user entered) 2410 HenryLC: 7.1e-007 atm-m3/mole (user entered) 2411 Log Kaw: -4.537 (air/water part.coef.) 2412 2413 LogKow : 4.73 (exp database) 2414 LogKow : 4.84 (KowWin estimate) 2415 Henry LC: 1.26e-006 atm-m3/mole (exp database) 2416 Henry LC: 4.22e-008 atm-m3/mole (HenryWin bond estimate) 2417 2418 Log Koa (octanol/air) estimate: 10.603 (from KowWin/HenryWin) 2419 2420 2421 2422 BIOWIN (v4.10) Program Results: 2423 \_\_\_\_\_ 2424 SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c22425 CHEM : Benzyl butyl phthalate 2426 MOL FOR: C19 H20 O4 2427 MOL WT : 312.37 2428 ----- BIOWIN v4.10 Results -----2429 2430 Biowin1 (Linear Model Prediction) : Biodegrades Fast 2431 Biowin2 (Non-Linear Model Prediction): Biodegrades Fast Biowin2 (Non Effect Float Floaterion): Broadgrades Fast Biowin3 (Ultimate Biodegradation Timeframe): Weeks 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 2432 2433 2434 2435 2436 2437 Ready Biodegradability Prediction: YES 2438 2439 2440 TYPE | NUM | Biowin1 FRAGMENT DESCRIPTION | COEFF | VALUE 2441 \_\_\_\_\_\_ 2442 Frag | 1 | Linear C4 terminal chain [CCC-CH3] | 0.1084 | 0.1084 2443 Frag | 2 | Ester [-C(=0)-O-C] | 0.1742 | 0.3484 

 Frag
 1
 Unsubstituted phenyl group (C6H5-)
 0.1281
 0.1281

 2444 2445 MolWt| \* | Molecular Weight Parameter | -0.1487 2446 Const| \* | Equation Constant | 0.7475 2448 RESULT | Biowin1 (Linear Biodeg Probability) | | 1.1837 2449 \_\_\_\_\_\_\_ 2450 2451 2452 TYPE | NUM | Biowin2 FRAGMENT DESCRIPTION | COEFF | VALUE 2453 

Frag   1 Frag   2 Frag   1 MolWt  *	<pre>Linear C4 terminal chain [CCC-CH3] Ester [-C(=O)-O-C] Unsubstituted phenyl group (C6H5-) Molecular Weight Parameter</pre>	1.8437   4.0795   1.7991 	1.8437   8.1590   1.7991   -4.4356
RESULT	=+====================================	+========   !	+=====================================
A Probabi A Probabi	ity Greater Than or Equal to 0.5 indicates> ity Less Than 0.5 indicates> Does NOT Biode	Biodegrade grade Fast	es Fast
TYPE   NU	Biowin3 FRAGMENT DESCRIPTION	+	+   VALUE
Frag   1 Frag   2 Frag   1 MolWt  * Const  *	<pre>  Linear C4 terminal chain [CCC-CH3]   Ester [-C(=O)-O-C]   Unsubstituted phenyl group (C6H5-)   Molecular Weight Parameter   Equation Constant</pre>	0.2983   0.1402   0.0220 	0.2983   0.2804   0.0220   -0.6903   3.1992
======= RESULT ========	=+====================================	+======   +============	+========   3.1096 +=======
+	-+	+	+
TYPE   NU	Biowin4 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag   1 Frag   2 Frag   1 MolWt  * Const  *	<pre>Linear C4 terminal chain [CCC-CH3] Ester [-C(=O)-O-C] Unsubstituted phenyl group (C6H5-) Molecular Weight Parameter Equation Constant</pre>	0.2691   0.2290   0.0049   	0.2692   0.4579   0.0049   -0.4507   3.8477
RESULT	=+====================================	+======	+======================================
Result Cl (Primary + TYPE   NU	ssification: 5.00 -> hours 4.00 -> days & Ultimate) 2.00 -> months 1.00 -> longe -+ Biowin5 FRAGMENT DESCRIPTION	3.00 -> r +	weeks
Frag   2 Frag   1 Frag   9 Frag   1 Frag   3 MolWt  * Const  *	<pre>Ester [-C(=O)-O-C] Aromatic-CH2 Aromatic-H Methyl [-CH3] -CH2- [linear] Molecular Weight Parameter Equation Constant</pre>	0.2319   0.0268   0.0004   0.0399   0.0255 	0.4638   0.0268   0.0036   0.0399   0.0399   0.0766   -0.4926   0.5544
 RESULT 	-+Biowin5 (MITI Linear Biodeg Probability) +=+==================================	+	+=====================================
+ TYPE   NU	-+Biowin6 FRAGMENT DESCRIPTION	+	+
 Frag   2 Frag   1	<pre>-+</pre>	+   1.5833   -0.0366	

Frag   Frag   Frag   MolWt	9 1 3 *	Aromatic-H   Methyl [-CH3]   -CH2- [linear]   Molecular Weight Parameter	0.0342 0.2351 0.2345	0.3077 0.2351 0.7035 -5.4040
RESU	'LT	Biowin6 (MITI Non-Linear Biodeg Probability)		0.6535
A Prob A Prob	abili <sup>.</sup> abili	ty Greater Than or Equal to 0.5 indicates> ty Less Than 0.5 indicates> NOT Readily De	Readily Degradable	egradable
TYPE	NUM	Biowin7 FRAGMENT DESCRIPTION	COEFF	VALUE
Frag   Frag   Frag   Frag   Frag   Frag   Const	1 2 1 9 1 3	<pre>Linear C4 terminal chain [CCC-CH3] Ester [-C(=O)-O-C] Unsubstituted phenyl group (C6H5-) Aromatic-CH2 Aromatic-H Methyl [-CH3] -CH2- [linear] Equation Constant</pre>	-0.3177   0.1719   0.2182   -0.0073   -0.0954   -0.0796   0.0260	-0.3177   0.3437   0.2182   -0.0073   -0.8589   -0.0796   0.0780   0.8361
====== RESU	====- 'LT	+=====================================	+======================================	+========   0.2124
Criter model) "weeks the pr satisf is bas (see H degrad Evalua	ia fo: resu " AND edict ied, ed on ed on elp). ation	r the YES or NO prediction: If the Biowin3 ( It is "weeks" or faster (i.e. "days", "days t the Biowin5 (MITI linear model) probability ion is YES (readily biodegradable). If this the prediction is NO (not readily biodegradab application of Bayesian analysis to ready bi Biowin5 and 6 also predict ready biodegrada in the OECD301C test only; using data from t and Research Institute Japan (CERIJ) database	ultimate su o weeks", o is >= 0.5, condition f le). This odegradation bility, but he Chemical	trvey then is not method on data t for ls
BioHCwi	n (v1	.01) Program Results:		
SMILES CHEM MOL FOR MOL WT	: O=C : Ben: : C19 : 312	(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c2 zyl butyl phthalate H20 O4 .37 BioHCwin v1.01 Results		
NO Es (Co	timat ntain:	e Possible Structure NOT a Hydrocarbon s atoms other than C, H or S (-S-))		

```
2568
2569
      AEROWIN Program (v1.00) Results:
2570
      _____
2571
       Sorption to aerosols (25 Dec C) [AEROWIN v1.00]:
2572
       Vapor pressure (liquid/subcooled): 0.0011 Pa (8.25E-006 mm Hg)
2573
       Log Koa (Koawin est ): 9.267
2574
        Kp (particle/gas partition coef. (m3/ug)):
2575
            Mackay model
                                  : 0.00273
2576
            Octanol/air (Koa) model: 0.000454
2577
        Fraction sorbed to airborne particulates (phi):
2578
            Junge-Pankow model : 0.0897
2579
            Mackay model
                                 : 0.179
2580
            Octanol/air (Koa) model: 0.035
2581
2582
2583
      AOP Program (v1.92) Results:
2584
      _____
2585
      SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c2
2586
      CHEM : Benzyl butyl phthalate
2587
      MOL FOR: C19 H20 O4
2588
     MOL WT : 312.37
2589
      ----- SUMMARY (AOP v1.92): HYDROXYL RADICALS (25 deg C) ------
2590
      Hydrogen Abstraction = 6.0617 \text{ E}-12 \text{ cm}3/\text{molecule-sec}
      Reaction with N, S and -OH = 0.0000 E-12 cm3/molecule-sec
2591
2592
      Addition to Triple Bonds = 0.0000 E-12 cm3/molecule-sec
2593
      Addition to Olefinic Bonds = 0.0000 E-12 cm3/molecule-sec
2594
      **Addition to Aromatic Rings = 4.9875 E-12 cm3/molecule-sec
2595
     Addition to Fused Rings = 0.0000 E-12 cm3/molecule-sec
2596
2597
        OVERALL OH Rate Constant = 11.0492 E-12 cm3/molecule-sec
2598
        HALF-LIFE = 0.968 Days (12-hr day; 1.5E6 OH/cm3)
2599
        HALF-LIFE = 11.616 Hrs
2600
      ..... ** Designates Estimation(s) Using ASSUMED Value(s)
2601
      ----- SUMMARY (AOP v1.91): OZONE REACTION (25 deg C) ------
2602
2603
                    ***** NO OZONE REACTION ESTIMATION ******
2604
                    (ONLY Olefins and Acetylenes are Estimated)
2605
2606
      Experimental Database: NO Structure Matches
2607
      Fraction sorbed to airborne particulates (phi):
2608
       0.134 (Junge-Pankow, Mackay avg)
2609
        0.035 (Koa method)
2610
          Note: the sorbed fraction may be resistant to atmospheric oxidation
2611
2612
2613
2614
2615
      KOCWIN Program (v2.00) Results:
2616
      _____
2617
      SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c2
2618
      CHEM : Benzyl butyl phthalate
2619
      MOL FOR: C19 H20 O4
2620
      MOL WT : 312.37
2621
2622
      _____
2623
      Experimental Database Structure Match:
2624
      Name : BENZYL BUTYL PHTHALATE
```

2625 CAS Num : 000085-68-7 2626 Exp LogKoc: 3.72 2627 Exp Ref : Schuurmann,G et al (2006); SRC (1991) 2628 2629 ----- KOCWIN v2.01 Results ------2630 2631 Koc Estimate from MCI: 2632 2633 First Order Molecular Connectivity Index ..... : 11.220 2634 Non-Corrected Log Koc (0.5213 MCI + 0.60) ..... : 6.4485 2635 Fragment Correction(s): 2636 2 Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -2.5939 2637 Corrected Log Koc ..... : 3.8546 2638 2639 Estimated Koc: 7155 L/kg <======= 2640 2641 Koc Estimate from Log Kow: 2642 \_\_\_\_\_ 2643 Log Kow (User entered ) ..... 4.73 2644 Non-Corrected Log Koc (0.55313 logKow + 0.9251) .... : 3.5414 2645 Fragment Correction(s): 2646 2 Ester (-C-CO-O-C-) or (HCO-O-C) ..... : -0.1312 2647 Corrected Log Koc ..... : 3.4102 2648 2649 Estimated Koc: 2572 L/kg <======== 2650 2651 2652 2653 2654 HYDROWIN Program (v2.00) Results: 2655 \_\_\_\_\_ 2656 SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c2 2657 CHEM : Benzyl butyl phthalate 2658 MOL FOR: C19 H20 O4 2659 MOL WT : 312.37 2660 ----- HYDROWIN v2.00 Results -----2661 2662 2663 NOTE: Fragment(s) on this compound are NOT available from the fragment 2664 library. Substitute(s) have been used!!! Substitute R1, R2, R3, 2665 or R4 fragments are marked with double astericks "\*\*". 2666 2667 \*\* R1: -Phenyl ESTER: R1-C (=0) -O-R2 2668 R2: -CH2-Phenyl 2669 NOTE: Ortho-position fragments(s) on Phenyl ring(s) are NOT CONSIDERED!! 2670 Kb hydrolysis at atom # 2: 1.264E-001 L/mol-sec 2671 2672 ESTER: R1-C (=0) -0-R2 R1: -Phenyl 2673 R2: n-Butyl-2674 Kb hydrolysis at atom # 16: 3.204E-002 L/mol-sec 2675 2676 Total Kb for pH > 8 at 25 deg C : 1.585E-001 L/mol-sec 2677 Kb Half-Life at pH 8: 50.617 days 2678 Kb Half-Life at pH 7: 1.386 years 2679 2680 2681

```
2682
2683
     BCFBAF Program (v3.01) Results:
2684
     _____
2685
     SMILES : O=C(OCc(cccc1)c1)c(c(ccc2)C(=0)OCCCC)c2
2686
     CHEM : Benzyl butyl phthalate
2687
     MOL FOR: C19 H20 O4
2688
     MOL WT : 312.37
2689
     ----- BCFBAF v3.01 -----
2690
     Summary Results:
     Log BCF (regression-based estimate): 2.79 (BCF = 614 L/kg wet-wt)
2691
      Biotransformation Half-Life (days) : 0.0354 (normalized to 10 g fish)
2692
2693
      Log BAF (Arnot-Gobas upper trophic): 1.60 (BAF = 40.1 L/kg wet-wt)
2694
2695
     Experimental BCF-kM Database Structure Match:
2696
     _____
      Name : 1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester
2697
2698
     CAS Num : 000085-68-7
      Log BCF : 1.2129 (BCF = 16.3 L/kg wet-wt)
2699
      BCF Data : BCF NonIonic Training Set
2700
2701
      Log Bio HL: -1.029 (Bio Half-life = 0.0935 days)
2702
      Bio Data : kM Training Set
2703
2704
     Log Kow (experimental): 4.73
2705
     Log Kow used by BCF estimates: 4.73 (user entered)
2706
2707
     Equation Used to Make BCF estimate:
2708
      Log BCF = 0.6598 \log Kow - 0.333 + Correction
2709
2710
         Correction(s):
                                   Value
2711
          No Applicable Correction Factors
2712
2713
       Estimated Log BCF = 2.788 (BCF = 613.6 L/kg wet-wt)
2714
2715
     _____
2716
     Whole Body Primary Biotransformation Rate Estimate for Fish:
2717
     _____
2718
    2719
     TYPE | NUM | LOG BIOTRANSFORMATION FRAGMENT DESCRIPTION | COEFF | VALUE
2720
     _____
2721
     Frag | 1 | Linear C4 terminal chain [CCC-CH3]
                                              | 0.0341 | 0.0341
2722
    Frag | 2 | Ester [-C(=0)-O-C]
                                                | -0.7605 | -1.5211
2723
     Frag | 1 | Unsubstituted phenyl group (C6H5-) | -0.6032 | -0.6032
     Frag | 1 | Aromatic-CH2
2724
                                                | -0.3365 | -0.3365
2725
     Frag | 9 | Aromatic-H
                                                | 0.2664 | 2.3974
2726
    Frag | 1 | Methyl [-CH3]
                                                | 0.2451 | 0.2451
2727
     Frag | 3 | -CH2- [linear]
                                                | 0.0242 | 0.0726
     Frag | 2 | Benzene
2728
                                                | -0.4277 | -0.8555
2729
     L Kow| * | Log Kow = 4.73 (user-entered ) | 0.3073 | 1.4537
    MolWt| * | Molecular Weight Parameter |
Const| * | Equation Constant |
2730
                                                        | -0.8010
2731
                                                        | -1.5371
2732
    RESULT | LOG Bio Half-Life (days) |
RESULT | Bio Half-Life (days) |
2733
                                                       | -1.4514
2734
                                                        | 0.03537
2735
      NOTE | Bio Half-Life Normalized to 10 g fish at 15 deg C |
2736
     2737
```

2739 kM (Rate Constant): 19.6 /day (10 gram fish) 2740 kM (Rate Constant): 11.02 /day (100 gram fish) 2741 kM (Rate Constant): 6.197 /day (1 kg fish) 2742 kM (Rate Constant): 3.485 /day (10 kg fish) 2743 2744 Note: For Arnot-Gobas BCF & BAF Methods, Experimental Km Half-Life Used: 2745 Exp Km Half-Life = -1.029 days (Rate Constant = 7.41/ day) 2746 Arnot-Gobas BCF & BAF Methods (including biotransformation rate estimates): 2747 Estimated Log BCF (upper trophic) = 1.603 (BCF = 40.08 L/kg wet-wt) 2748 Estimated Log BAF (upper trophic) = 1.603 (BAF = 40.08 L/kg wet-wt) Estimated Log BCF (mid trophic) = 1.735 (BCF = 54.36 L/kg wet-wt) Estimated Log BAF (mid trophic) = 1.737 (BAF = 54.54 L/kg wet-wt) 2749 2750 2751 Estimated Log BCF (lower trophic) = 1.775 (BCF = 59.62 L/kg wet-wt) 2752 Estimated Log BAF (lower trophic) = 1.796 (BAF = 62.46 L/kg wet-wt) 2753 2754 Arnot-Gobas BCF & BAF Methods (assuming a biotransformation rate of zero): 2755 Estimated Log BCF (upper trophic) = 3.684 (BCF = 4827 L/kg wet-wt) 2756 Estimated Log BAF (upper trophic) = 4.577 (BAF = 3.777e+004 L/kg wet-wt) 2757 2758 2759 2760 2761 2762 Volatilization From Water 2763 \_\_\_\_\_ 2764 2765 Chemical Name: Benzyl butyl phthalate 2766 2767 Molecular Weight : 312.37 g/mole Water Solubility : 2.69 ppm Vapor Pressure : 8.25E-006 mm Hg 2768 2769 2770 Henry's Law Constant: 7.1E-007 atm-m3/mole (entered by user) 2771 2772 RIVER LAKE 2773 \_\_\_\_\_ \_\_\_\_\_ Water Depth (meters): 1 Wind Velocity (m/sec): 5 2774 1 2775 0.5 2776 Current Velocity (m/sec): 1 0.05 2777 HALF-LIFE (hours) : 1459 2778 1.607E+004 2779 HALF-LIFE (days ) : 60.8 669.5 2780 HALF-LIFE (years) : 0.1665 1.833 2781 2782 2783 STP Fugacity Model: Predicted Fate in a Wastewater Treatment Facility 2784 2785 (using Biowin/EPA draft method) 2786 PROPERTIES OF: Benzyl butyl phthalate 2787 \_\_\_\_\_ 2788 312.37 Molecular weight (g/mol) 2789 Aqueous solubility (mg/l) 2.69 2790 Vapour pressure (Pa) 0.00109991 2791 1.08553E-008 (atm) 2792 (mm Hg) 8.25E-006 2793 Henry 's law constant (Atm-m3/mol) 7.1E-007 2794 Air-water partition coefficient 2.90369E-005 2795 Octanol-water partition coefficient (Kow) 53703.2

Log Kow Biomass to w	water partiti	on coefficie	nt	4	.73 0741.4
Biodeg rate (h):	[deg C] constants (h	^-1),half li	fe in bioma	ss (h) an	d in 2000 mg/
-]	Primary tank	0.07	9.5	6	10.00
-7	Aeration tank	0.73	0.9	6	1.00
- 2	Settling tank	0.73	0.9	6	1.00
STP Overal	l Chemical Ma	ss Balance:			
		g/h	1	mol/h	percent
Influent		1.00E+00	1 3	.2E-002	100.00
Primarv slu	dae	1.82E+00	0 5	.8E-003	18.20
Waste sludge	e	1.14E-00	2 3	.7E-005	0.11
Primarv vola	atilization	5.44E-00	5 1	.7E-007	0.00
Settling vo	latilization	1.33E-00	6 4	.3E-009	0.00
Aeration of:	f gas	4.08E-00	6 1	.3E-008	0.00
Primary bio	degradation	5 565+00	0 1	8E-002	55 63
Settling hi	odegradation	1 50F-00	1 1	8E-004	1 50
Aeration bio	odegradation	2.44E+00	0 7	.8E-003	24.41
Final water	effluent	1.45E-00	2 4	.6E-005	0.14
	- 1		0 2		
rotal remova	d⊥	9.99E+00	0 3	.2E-002	99.80
Chem Name Molecular Henry's LG Vapor Pres Log Kow Soil Koc N Air	: BBP Wt: 312.37 C : 7.61e-00 ss : 8.25e-00 : 4.73 (u : 7.24e+00 Mass Amount (percent) 3.32	7 atm-m3/mol 6 mm Hg (us ser-entered) 4 (user-ent Half-Life (hr) 23.3	e (user-entered) er-entered) ered) Emission (kg/hr) 1000	= ered) s	
Water	21.6	120	1000		
Soil	59.5	240	1000		
Sediment	15.6	1.08e+0	<mark>03 0</mark>		
	Fugacity	Reaction	Advection	Reactic	n Advectio
	(atm)	(kg/hr)	(kg/hr)	(percen	t) (percent
Air	1.52e-011	643	216	21.4	7.21
Water	1.54e-012	813	141	27.1	4.69
Soil	3.02e-014	1.12e+003	0	37.3	0
Sediment	3.56e-013	65.3	2.03	2.18	0.0678
Persister	nce Time: 217	hr			
Reaction	Time: 247	hr			

1.82e+003 hr 2853 Advection Time: 2854 Percent Reacted: 88 2855 Percent Advected: 12 2856 2857 Water Compartment Percents: 2858 \_\_\_\_\_ 2859 Mass Amount Half-Life Emissions 2860 (percent) (hr) (kg/hr) 2861 3.32 23.3 1000 Air 2862 Water 21.6 120 1000 2863 water (19.4)2864 biota (0.0522)2865 suspended sediment (2.11) 2866 Soil 59.5 1000 240 2867 Sediment 15.6 1.08e+003 0 2868 2869 Half-Lives (hr), (based upon user-entry): 2870 Air: 23.3 2871 Water: 120 2872 Soil: 240 2873 Sediment: 1080 2874 2875 Advection Times (hr): 2876 Air: 100 2877 Water: 1000 2878 Sediment: 5e+004 2879 2880 2881 Level III Fugacity Model (Full-Output): EQC Default 2882 Chem Name : BBP 2883 2884 Molecular Wt: 312.37 2885 Henry's LC : 7.61e-007 atm-m3/mole (user-entered) 2886 Vapor Press : 8.25e-006 mm Hg (user-entered) 2887 Log Kow : 4.73 (user-entered) 2888 Soil Koc : 2.2e+004 (EQC Model Default) 2889 2890 Mass Amount Half-Life Emissions 2891 (kg/hr) (percent) (hr) 2892 3.65 23.3 1000 Air 2893 Water 24.9 120 1000 2894 65.5 240 1000 Soil 2895 Sediment 5.96 1.08e+003  $\cap$ 2896 2897 Fugacity Reaction Advection Reaction Advection 2898 (kg/hr) (kg/hr) (percent) (atm) (percent) 2899 Air 1.52e-011 643 216 21.4 7.21 2900 Water 1.73e-012 851 147 28.4 4.91 2901 Soil 9.92e-014 1.12e+003 0 37.3 0 2902 Sediment 4.06e-013 22.6 0.705 0.754 0.0235 2903 2904 Persistence Time: 197 hr 2905 Reaction Time: 225 hr 2906 Advection Time: 1.62e+003 hr 2907 Percent Reacted: 87.9 2908 Percent Advected: 12.1 2909

	Mass Amount	Half-Life	Emissions	3	
	(percent)	(hr)	(kg/hr)		
Air	3.65	23.3	1000		
Water	24.9	120	1000		
water	(24)				
biota	(0.0645)				
susper	ided sediment	(0./94)	1000		
Soll	65.5	240	1000		
Seatmen	- 5.96	1.080+00	13 0		
Half-Liv	ves (hr), (bas	sed upon user-	entry):		
Air:	23.3				
Water	r: 120				
Soil	: 240				
Sedir	aent: 1080				
Advectio	on Times (hr):	:			
Air:	100				
Water	<b>:</b> 1000				
Sedir	nent: 5e+004				
	Fuqacity Modo	] (Full_Output	). Usor Kor	•	
=========		======================================	============	-	
Chem Name	≥ : BBP				
Chem Name Molecula:	> : BBP : Wt: 312.37				
Chem Name Molecula: Henry's 1	e : BBP c Wt: 312.37 GC : 7.61e-00	07 atm-m3/mole	e (user-ente	ered)	
Chem Name Molecula: Henry's 1 Vapor Pre	<ul> <li>BBP</li> <li>Wt: 312.37</li> <li>C : 7.61e-00</li> <li>ss : 8.25e-00</li> </ul>	07 atm-m3/mole 06 mm Hg (use	e (user-ente er-entered)	ered)	
Chem Name Molecular Henry's I Vapor Pre Log Kow	<pre>BBP Wt: 312.37 C : 7.61e-00 Sss : 8.25e-00 C : 4.73 (1)</pre>	07 atm-m3/mole 06 mm Hg (use 1ser-entered)	e (user-ente er-entered)	ered)	
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc	e : BBP c Wt: 312.37 LC : 7.61e-00 ess : 8.25e-00 : 4.73 (u : 7.24e+00	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente	e (user-ente er-entered) ered)	ered)	
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc	<pre>e : BBP c Wt: 312.37 LC : 7.61e-00 ess : 8.25e-00</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life	e (user-ente er-entered) ered) Emissions	ered)	
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc	<pre>BBP Wt: 312.37 C : 7.61e-00 BSS : 8.25e-00 C : 4.73 (u C : 7.24e+00 Mass Amount (percent)</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr)	e (user-ente er-entered) ered) Emissions (kg/hr)	ered)	
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air	<pre>BBP Wt: 312.37 C : 7.61e-0( sss : 8.25e-0(</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120	e (user-ente er-entered) ered) Emissions (kg/hr) 1000 0	ered)	
Chem Name Molecular Henry's 1 Vapor Pro Log Kow Soil Koc Air Water Soil	<pre>BBP Wt: 312.37 C : 7.61e-0( sss : 8.25e-0(</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240	e (user-ente er-entered) ered) Emissions (kg/hr) 1000 0	ered)	
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment	<pre>BBP Wt: 312.37 C : 7.61e-0( ss : 8.25e-0(</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00	e (user-ente er-entered) ered) Emissions (kg/hr) 1000 0 0 0	ered)	
Chem Name Molecular Henry's 1 Vapor Pre Log Kow Soil Koc Air Water Soil Sediment	<pre>BBP Wt: 312.37 C : 7.61e-0( sss : 8.25e-0(</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00	e (user-ente er-entered) ered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0	ered)	
Chem Name Molecular Henry's 1 Vapor Pre Log Kow Soil Koc Air Water Soil Sediment	<pre>e : BBP r Wt: 312.37 LC : 7.61e-0( ess : 8.25e-0(</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction	e (user-ente er-entered) ered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	ered)	Advection
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment	<pre></pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction (kg/hr)	e (user-ente er-entered) Emissions (kg/hr) 1000 0 3 0 Advection (kg/hr)	Reaction (percent)	Advection (percent)
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air	<pre>e : BBP r Wt: 312.37 LC : 7.61e-0( ess : 8.25e-0(</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction (kg/hr) 642	e (user-ente er-entered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Reaction (percent) 64.2	Advection (percent) 21.6
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air Water	<pre>e : BBP r Wt: 312.37 LC : 7.61e-0( ess : 8.25e-0(</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8	e (user-ente er-entered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Reaction (percent) 64.2 1.78	Advection (percent) 21.6 0.308
Chem Name Molecular Henry's I Vapor Pro Log Kow Soil Koc Air Water Soil Air Water Soil	<pre>e : BBP r Wt: 312.37 LC : 7.61e-0( ess : 8.25e-0(                 : 4.73 (1                 : 7.24e+0( Mass Amount                (percent)</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119	e (user-entered) ered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Reaction (percent) 64.2 1.78 11.9	Advection (percent 21.6 0.308 0
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air Water Soil Sediment	<pre>e : BBP r Wt: 312.37 LC : 7.61e-0( ess : 8.25e-0(         : 4.73 (1         : 7.24e+0( Mass Amount         (percent)         31.7         4.51         60.6         : 3.26 Fugacity         (atm)         1.52e-011         3.37e-014         3.21e-015         : 7.78e-015 </pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119 1.43	e (user-entered) ered) Emissions (kg/hr) 1000 0 0 3 0 Advection (kg/hr) 216 3.08 0 0.0445	Reaction (percent) 64.2 1.78 11.9 0.143	Advectio (percent 21.6 0.308 0 0.00445
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air Water Soil Sediment Persiste	<pre>BBP Wt: 312.37 C : 7.61e-0( sss : 8.25e-0(</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119 1.43 .2 hr	e (user-entered) ered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Reaction (percent) 64.2 1.78 11.9 0.143	Advectio (percent 21.6 0.308 0 0.00445
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air Water Soil Sediment Persiste Reaction	<pre>e : BBP r Wt: 312.37 LC : 7.61e-0( ess : 8.25e-0(                 : 4.73 (1                 : 7.24e+0( Mass Amount                (percent)</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119 1.43 .2 hr .3 hr	e (user-entered) ered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Reaction (percent) 64.2 1.78 11.9 0.143	Advectio (percent 21.6 0.308 0 0.00445
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air Water Soil Sediment Persiste Reaction Advectio	<pre>BBP Wt: 312.37 C : 7.61e-0( ss : 8.25e-0(                 : 4.73 (1                 : 7.24e+0( Mass Amount                (percent)</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119 1.43 .2 hr .3 hr 1 hr	e (user-entered) ered) Emissions (kg/hr) 1000 0 0 3 0 Advection (kg/hr) 216 3.08 0 0.0445	Reaction (percent) 64.2 1.78 11.9 0.143	Advectio (percent 21.6 0.308 0 0.00445
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air Water Soil Sediment Persiste Reaction Advection	<pre>e : BBP r Wt: 312.37 LC : 7.61e-0( ess : 8.25e-0(         : 4.73 (u         : 7.24e+0( Mass Amount         (percent)         31.7         4.51         60.6         3.26          Fugacity         (atm)         1.52e-011         3.37e-014         3.21e-015         7.78e-015 ence Time: 68.4 n Time: 87.5 n Time: 311 Reacted: 78.4 </pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-entered) 04 (user-entered) 123.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119 1.43 .2 hr .3 hr 1 hr .1	e (user-entered) ered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Reaction (percent) 64.2 1.78 11.9 0.143	Advectio (percent 21.6 0.308 0 0.00445
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air Water Soil Sediment Persiste Reaction Advectio Percent Percent	<pre>e : BBP r Wt: 312.37 LC : 7.61e-0( ess : 8.25e-0(</pre>	<pre>07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-entered) 04 (user-entered) 120 23.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119 1.43 .2 hr .3 hr 1 hr .1 .9</pre>	e (user-entered) ered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Reaction (percent) 64.2 1.78 11.9 0.143	Advectio (percent 21.6 0.308 0 0.00445
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air Water Soil Sediment Persiste Reaction Advection Percent	<pre>e : BBP r Wt: 312.37 LC : 7.61e-0( ess : 8.25e-0(</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119 1.43 .2 hr .3 hr 1 hr .1 .9	e (user-entered) ered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Reaction (percent) 64.2 1.78 11.9 0.143	Advection (percent 21.6 0.308 0 0.00445
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air Water Soil Sediment Persiste Reaction Advection Percent Percent Water Co	<pre>BBP Wt: 312.37 C : 7.61e-0( ess : 8.25e-0(</pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-ente Half-Life (hr) 23.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119 1.43 .2 hr .3 hr 1 hr .1 .9 rcents:	e (user-entered) ered) Emissions (kg/hr) 1000 0 3 0 Advection (kg/hr) 216 3.08 0 0.0445	Reaction (percent) 64.2 1.78 11.9 0.143	Advection (percent 21.6 0.308 0 0.00445
Chem Name Molecular Henry's I Vapor Pre Log Kow Soil Koc Air Water Soil Sediment Air Water Soil Sediment Persiste Reaction Advection Percent Percent Water Co	<pre></pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-entered) 04 (user-entered) 123.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119 1.43 .2 hr .3 hr 1 hr .1 .9 rcents:	e (user-entered) ered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Reaction (percent) 64.2 1.78 11.9 0.143	Advectio (percent 21.6 0.308 0 0.00445
hem Name olecular enry's l apor Pre og Kow oil Koc Air Nater Soil Sediment Air Persiste Reaction Advectio Percent Percent Mater Co	<pre></pre>	07 atm-m3/mole 06 mm Hg (use user-entered) 04 (user-entered) 04 (user-entered) 120 23.3 120 240 1.08e+00 Reaction (kg/hr) 642 17.8 119 1.43 .2 hr .3 hr 1 hr .1 .9 rcents:  Half-Life	e (user-entered) ered) Emissions (kg/hr) 1000 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	Reaction (percent) 64.2 1.78 11.9 0.143	Advectic (percent 21.6 0.308 0 0.00445

2967 2968 2969 2970	Air Water water biota	31.7 4.51 (4.06) (0.0109)	23.3 120	1000 0		
2971 2972 2973 2974	suspen Soil Sediment	ded sediment 60.6 3.26	(0.441) 240 1.08e+0	0 03 0		
2975 2976 2977 2978 2979 2980	Half-Liv Air: Water Soil: Sedim	es (hr), (bas 23.3 : 120 240 ent: 1080	sed upon user	-entry):		
2980 2981 2982 2983 2984 2985 2086	Advectio Air: Water Sedim	n Times (hr): 100 : 1000 ent: 5e+004	:			
2980 2987 2988	Level III F ========	ugacity Model	L (Full-Outpu	t): EQC Defa	ult =====	
2989 2990 2991 2992 2993 2994	Chem Name Molecular Henry's L Vapor Pre Log Kow Soil Koc	: BBP Wt: 312.37 C : 7.61e-00 ss : 8.25e-00 : 4.73 (1 : 2.2e+004	)7 atm-m3/mol )6 mm Hg (us user-entered) 4 (EQC Model	e (user-ente er-entered) Default)	red)	
2995 2996 2997		Mass Amount (percent)	Half-Life (hr)	Emissions (kg/hr)		
2998	Air	32.3	23.3	1000		
2999	Water	4.82	120	0		
3000	Soil	61.7	240	0		
3001 3002	Sediment	1.15	1.08e+0	03 0		
3003 3004		Fugacity	Reaction (kg/br)	Advection	Reaction	Advection
3005	Dir	1 52 = 011	(Kg/III) 642	216	(percenc) 64 2	(percenc) 21 6
3006	Water	379e-014	18 6	3 22	1 86	0 322
3007	Soil	1.06e-014	119	0	11.9	0
3008	Sediment	8.87e-015	0.495	0.0154	0.0495	0.00154
3009						
3010	Persiste	nce Time: 66.	.9 hr			
3011	Reaction	Time: 85	.7 hr			
3012	Advectio	n Time: 305	5 hr			
3013	Percent	Reacted: 78	.1			
3014	Percent	Advected: 21	. 9			
3015						
3016	Water Co	mpartment Per	ccents:			
3017						
3018		Mass Amount	Half-Life	Emissions		
3019		(percent)	(hr)	(kg/hr)		
3020 2021	Alr	32.3	23.3	1000		
3021	Water	4.82	120	0		
3022	water	(4.65)				
5045	DIOLA	$(\cup \cdot \cup \perp \angle \cup)$				
3024 suspended sediment (0.154) 3025 Soil 61.7 240 0 3026 Sediment 1.15 1.08e+003 0 3027 3028 Half-Lives (hr), (based upon user-entry): 3029 Air: 23.3 3030 Water: 120 3031 Soil: 240 3032 Sediment: 1080 3033 3034 Advection Times (hr): 3035 Air: 100 3036 Water: 1000 3037 Sediment: 5e+004 3038 3039 3040 Level III Fugacity Model (Full-Output): User Koc 3041 \_\_\_\_\_ Chem Name : BBP 3042 3043 Molecular Wt: 312.37 3044 Henry's LC : 7.61e-007 atm-m3/mole (user-entered) 3045 Vapor Press : 8.25e-006 mm Hg (user-entered) Log Kow : 4.73 (user-entered) 3046 3047 Soil Koc : 7.24e+004 (user-entered) 3048 3049 Mass Amount Half-Life Emissions 3050 (hr) (kg/hr) (percent) 23.3 3051 0.00876 Air 0 3052 58 120 1000 Water 3053 Soil 0.0167 240 0 3054 Sediment 41.9 1.08e+003 0 3055 3056 Fugacity Reaction Advection Reaction Advection 3057 (atm) (kg/hr) (kg/hr) (percent) (percent) 0.618 795 3058 1.47e-014 Air 0.208 0.0618 0.0208 1.51e-012 138 3059 Water 79.5 13.8 3.09e-018 0.115 3060 Soil 0 0.0115 0 63.8 1.99 3061 Sediment 3.48e-013 6.38 0.199 3062 3063 Persistence Time: 237 hr 3064 Reaction Time: 276 hr 3065 Advection Time: 1.7e+003 hr 3066 Percent Reacted: 86 3067 Percent Advected: 14 3068 3069 Water Compartment Percents: 3070 \_\_\_\_\_ 3071 Half-Life Emissions Mass Amount 3072 (hr) (percent) (kq/hr) 3073 0.00876 23.3 0 Air 3074 Water 120 58 1000 3075 water (52.2)3076 biota (0.14) 3077 suspended sediment (5.68) 3078 Soil 0.0167 240 0 3079 Sediment 41.9 1.08e+003 0 3080

3081 Half-Lives (hr), (based upon user-entry): 3082 23.3 Air: 3083 120 Water: 3084 Soil: 240 3085 Sediment: 1080 3086 3087 Advection Times (hr): 3088 Air: 100 3089 Water: 1000 3090 Sediment: 5e+004 3091 3092 3093 Level III Fugacity Model (Full-Output): EQC Default 3094 \_\_\_\_\_ 3095 Chem Name : BBP 3096 Molecular Wt: 312.37 3097 Henry's LC : 7.61e-007 atm-m3/mole (user-entered) 3098 Vapor Press : 8.25e-006 mm Hg (user-entered) 3099 Log Kow : 4.73 (user-entered) 3100 Soil Koc : 2.2e+004 (EQC Model Default) 3101 3102 Half-Life Mass Amount Emissions 3103 (percent) (hr) (kq/hr) 3104 Air 0.0131 23.3 0 3105 Water 80.7 120 1000 3106 0.025 Soil 240 0 3107 Sediment 19.3 1.08e+003 0 3108 3109 Fugacity Reaction Advection Reaction Advection 3110 (kg/hr) (kg/hr) (percent) (percent) (atm) 3111 0.233 0.0694 Air 1.64e-014 0.694 0.0233 3112 Water 1.69e-012 832 144 83.2 14.4 3113 Soil 1.14e-017 0.129 0.0129 0 0 Sediment 3.97e-013 0.069 3114 22.1 0.69 2.21 3115 3116 Persistence Time: 179 hr 3117 Reaction Time: 209 hr 3118 Advection Time: 1.23e+003 hr Percent Reacted: 85.5 3119 3120 Percent Advected: 14.5 3121 3122 Water Compartment Percents: 3123 \_\_\_\_\_ 3124 Half-Life Emissions Mass Amount 3125 (percent) (hr) (kg/hr) 3126 0.0131 23.3 0 Air 3127 120 Water 80.7 1000 3128 water (77.9)3129 biota (0.209)3130 suspended sediment (2.57) 3131 Soil 0.025 240 0 3132 Sediment 19.3 1.08e+003 Ω 3133 3134 Half-Lives (hr), (based upon user-entry): 3135 Air: 23.3 3136 Water: 120 3137 240 Soil:

3138 Sediment: 1080 3139 3140 Advection Times (hr): 3141 Air: 100 1000 3142 Water: 3143 Sediment: 5e+004 3144 3145 3146 Level III Fugacity Model (Full-Output): User Koc 3147 3148 Chem Name : BBP 3149 Molecular Wt: 312.37 3150 Henry's LC : 7.61e-007 atm-m3/mole (user-entered) 3151 Vapor Press : 8.25e-006 mm Hg (user-entered) 3152 Log Kow : 4.73 (user-entered) 3153 : 7.24e+004 (user-entered) Soil Koc 3154 3155 Mass Amount Half-Life Emissions 3156 (percent) (hr) (kg/hr) 3157 Air 6.23e-005 23.3 120 0 3158 0.00337 0 Water 3159 Soil 100 240 1000 Sediment 0.00243 3160 1.08e+0030 3161 3162 Fugacity Reaction Advection Reaction Advection (atm)(kg/hr)(kg/hr)(percent)Air1.52e-0160.006410.002160.0006410.000216Water1.28e-0160.06730.01170.006730.00117Soil2.7e-0141e+00301000 3163 3164 3165 3166 Sediment 2.95e-017 0.0054 0.000168 0.00054 1.68e-005 3167 3168 3169 Persistence Time: 346 hr 3170 Reaction Time: 346 hr 3171 Advection Time: 2.48e+007 hr Percent Reacted: 100 3172 3173 Percent Advected: 0.0014 3174 3175 Water Compartment Percents: 3176 \_\_\_\_\_ 3177 Half-Life Mass Amount Emissions 3178 (percent) (hr) (kq/hr) 3179 6.23e-005 23.3 0 Air Water 120 3180 0.00337 0 3181 water (0.00303) biota (8.13e-006) 3182 3183 suspended sediment (0.000329) 3184 Soil 100 240 1000 3185 Sediment 0.00243 1.08e+003 0 3186 3187 Half-Lives (hr), (based upon user-entry): 3188 Air: 23.3 120 3189 Water: 3190 Soil: 240 3191 Sediment: 1080 3192 3193 Advection Times (hr): 3194 Air: 100

3195 Water: 1000 3196 Sediment: 5e+004 3197 3198 3199 Level III Fugacity Model (Full-Output): EQC Default 3200 \_\_\_\_\_ 3201 Chem Name : BBP 3202 Molecular Wt: 312.37 3203 Henry's LC : 7.61e-007 atm-m3/mole (user-entered) 3204 Vapor Press : 8.25e-006 mm Hg (user-entered) 3205 Log Kow : 4.73 (user-entered) 3206 Soil Koc : 2.2e+004 (EOC Model Default) 3207 3208 Half-Life Emissions Mass Amount 3209 (kg/hr) (percent) (hr) 3210 0.000204 23.3 0 Air 3211 0.00828 120 0 Water 3212 Soil 100 240 1000 3213 Sediment 0.00198 1.08e+003 0 3214 3215 Reaction Advection Reaction Advection Fugacity 3216 (kg/hr) (percent) (percent) (atm) (kg/hr) 0.00211 0.0166 0.000708 3217 0.00708 Air 4.99e-016 0.0211 3218 0.166 Water 3.37e-016 0.0287 0.00287 3219 Soil 8.86e-014 1e+003 100 0 0 3220 0.000137 0.00044 Sediment 7.9e-017 0.0044 1.37e-005 3221 3222 Persistence Time: 346 hr 3223 Reaction Time: 346 hr 3224 Advection Time: 9.65e+006 hr 3225 Percent Reacted: 100 3226 Percent Advected: 0.00359 3227 3228 Water Compartment Percents: 3229 \_\_\_\_\_ 3230 Mass Amount Half-Life Emissions 3231 (percent) (hr) (kg/hr) 3232 0.000204 23.3 0 Air 0.00828 3233 Water 0 120 3234 water (0.008) 3235 biota (2.15e-005)3236 suspended sediment (0.000264) 3237 Soil 100 240 1000 3238 Sediment 0.00198 1.08e+003 0 3239 3240 Half-Lives (hr), (based upon user-entry): 3241 Air: 23.3 3242 Water: 120 3243 Soil: 240 3244 Sediment: 1080 3245 3246 Advection Times (hr): 3247 Air: 100 3248 Water: 1000 3249 Sediment: 5e+004 3250 3251

Henry's L Vapor Pre Log Kow Soil Koc	c : 7.61e-00 ss : 8.25e-00 : 4.73 (u : 7.24e+00	)7 atm-m3/mol )6 mm Hg (us user-entered) )4 (user-ent	e (user-ente er-entered) ered)	ered)	
Air Water Soil Sediment	Mass Amount (percent) 7.08 46.1 13.5 33.3	Half-Life (hr) 23.3 120 240 1.08e+0	Emissions (kg/hr) 1000 1000 0 03 0		
Dir	Fugacity (atm) 1 52e-011	Reaction (kg/hr) 643	Advection (kg/hr) 216	Reaction (percent)	Adv (pe
Water	1.54e-012	81.3	141	40.7	7.
Soil	3.22e-015	119	0	5.97	0
Sediment	3.56e-013	65.3	2.03	3.26	0.
Water Co	mpartment Per	cents:			
Water Co  Air Water	Mass Amount (percent) 7.08 46.1	Half-Life (hr) 23.3 120	Emissions (kg/hr) 1000 1000	5	
Water Co  Air Water water biota	mpartment Per  Mass Amount (percent) 7.08 46.1 (41.5) (0 111)	Half-Life (hr) 23.3 120	Emissions (kg/hr) 1000 1000	5	
Water Co  Air Water water biota suspen	mpartment Per Mass Amount (percent) 7.08 46.1 (41.5) (0.111) ded sediment	Half-Life (hr) 23.3 120 (4.51)	Emissions (kg/hr) 1000 1000		
Water Co  Air Water water biota suspen Soil	mpartment Per Mass Amount (percent) 7.08 46.1 (41.5) (0.111) ded sediment 13.5	Half-Life (hr) 23.3 120 (4.51) 240	Emissions (kg/hr) 1000 1000		
Water Co  Air Water water biota suspen Soil Sediment	mpartment Per Mass Amount (percent) 7.08 46.1 (41.5) (0.111) ded sediment 13.5 33.3	Half-Life (hr) 23.3 120 (4.51) 240 1.08e+0	Emissions (kg/hr) 1000 1000 0 03 0		
Water Co  Air Water biota suspen Soil Sediment Half-Liv Air: Water Soil: Sedim	<pre>mpartment Per Mass Amount (percent) 7.08 46.1 (41.5) (0.111) ded sediment 13.5 33.3 es (hr), (bas 23.3 : 120 240 ent: 1080</pre>	Half-Life (hr) 23.3 120 (4.51) 240 1.08e+0 sed upon user	Emissions (kg/hr) 1000 1000 0 03 0 -entry):		
Water Co Air Water water biota suspen Soil Sediment Half-Liv Air: Water Soil: Sedim Advectio Air: Water Sedim	<pre>mpartment Per Mass Amount (percent) 7.08 46.1 (41.5) (0.111) ded sediment 13.5 33.3 es (hr), (bas 23.3 : 120 240 ent: 1080 n Times (hr): 100 : 1000 ent: 5e+004</pre>	Half-Life (hr) 23.3 120 (4.51) 240 1.08e+0 sed upon user	Emissions (kg/hr) 1000 1000 0 03 0 -entry):		

M Air Wator	lass Amount (percent) 8.81 60	Half-Life (hr) 23.3	Emission (kg/hr) 1000	S	
Soil Sediment	16.8 14.4	240 1.08e+0	003		
	Fugacity	Reaction (kg/hr)	Advection	Reaction	Advectic
Air	1.52e-011	643	216	32.2	10.8
Water	1.73e-012	851	147	42.5	7.36
Soil	1.06e-014	119	0	5.97	0
Sediment	4.06e-013	22.6	0.705	1.13	0.0353
Persisten	ce Time. 123	} hr			
Reaction	Time: 150	) hr			
Advection	Time: 674	l hr			
Percent R	eacted: 81.	8			
Percent A	dvected: 18.	2			
Water Com	partment Per	cents:			
M	lass Amount	Half-Life	Emission	S	
	(percent)	(hr)	(kg/hr)		
Air	8.81	23.3	1000		
Water	60	120	1000		
water	(57.9)				
biota	(0.156)	(1.01)			
suspend	led sediment	(1.91)	0		
Soll	16.8	240	0		
Sediment	14.4	1.08e+0	03 0		
Half-Live	s (hr), (bas	sed upon user	r-entry):		
Air:	23.3				
Water:	120				
Soil:	240				
Sedime	nt: 1080				
Advection	Times (hr):				
Air:	100				
Water:	1000				
Sedime	nt: 5e+004				
]					
evel III Fu	gacity Model	_ (Full-Outpu	it): User Ko 	C _	
Chem Name	• BBP			_	
Molecular	Wt: 312.37				
Henry's LC	: 7.61e-00	)7 atm-m3/mol	le (user-ent	ered)	
Vapor Pres	s : 8.25e-00	)6 mm Hg (us	ser-entered)		
Log Kow	: 4.73 (u	ser-entered)	,		

	Mass Amount	Half-Life	Emissions	5	
	(percent)	(hr)	(kg/hr)		
Air	5.21	23.3	1000		
Water	0.745	120	0		
Soll	93.5	240	1000		
Sediment	t 0.538	1.08e+0	03 0		
	Fugacity	Reaction	Advection	Reaction	Advection
	(atm)	(kg/hr)	(kg/hr)	(percent)	(percent)
Air	1.52e-011	642	216	32.1	10.8
Water	3.39e-014	17.8	3.09	0.892	0.154
Soil	3.02e-014	1.12e+003	0	56	0
Sediment	z 7.81e-015	1.43	0.0446	0.0716	0.00223
Persiste	ence Time: 20	7 hr			
Reaction	n Time: 233	3 hr			
Advectio	on Time: 1.8	89e+003 hr			
Percent	Reacted: 89				
Percent	Advected: 11				
Watan O	D				
water Co	Smpartment Per	rcents:			
	Mass Amount	Half-Iifo	Emission	3	
	(percent)	(hr)	(ka/hr)	<u>,</u>	
Air	5.21	23.3	1000		
Water	0.745	120	0		
water	(0.671)	120	Ũ		
biota	(0.0018)				
susper	nded sediment	(0.0729)			
Soil	93.5	240	1000		
Sediment	c 0.538	1.08e+0	0 0 0		
Half-Lix	ves (hr), (bas	sed upon user	-entry).		
Air:	23.3	bed apon aber	enery,.		
Wate	r: 120				
Soil	240				
Sedir	ment: 1080				
Ndreat -	on Timor (br)				
Auvectio	100 1100	•			
	100 r• 1000				
vale Sadir	1 + 1000				
Deall					
Level III H	Eugacity Model	l (Full-Outpu	it): EQC Defa	ault	
Chem Name	e : BBP				
Molecular	r Wt: 312.37				
Henry's l	LC : 7.61e-00	07 atm-m3/mol	e (user-ente	ered)	
Vapor Pre	ess : 8.25e-00	06 mm Hg (us	ser-entered)		
Log Kow	: 4.73 (1	user-entered)			
Soil Koc	: 2.2e+004	4 (EQC Model	. Default)		
	Mass Amount	Half-Tifo	Emission	3	
	(percent)	(hr)	(ka/hr)	ر	
Air	5.23	2:3.3	1000		

3423 3424 3425 3426	Water Soil Sediment	0.787 93.8 0.188	120 240 1.08e+0	0 1000 03 0		
3420 3427 3428 3429 3430 3431 3432	Air Water Soil Sediment	Fugacity (atm) 1.52e-011 3.82e-014 9.92e-014 8.95e-015	Reaction (kg/hr) 642 18.8 1.12e+003 0.499	Advection (kg/hr) 216 3.25 0 0.0156	Reaction (percent) 32.1 0.938 55.9 0.025	Advection (percent) 10.8 0.162 0 0.000778
3433 3434 3435 3436 3437 3438 3439 3440	Persisten Reaction Advection Percent R Percent A	ace Time: 207 Time: 232 a Time: 1.8 Reacted: 89 Advected: 11	7 hr 2 hr 38e+003 hr			
3441						
3442 3443 3444 3445 3446 3447	Air Water water biota	Iass Amount (percent) 5.23 0.787 (0.759) (0.00204)	Half-Life (hr) 23.3 120	Emissions (kg/hr) 1000 0	5	
3448 3449 3450 3451	suspend Soil Sediment	led sediment 93.8 0.188	(0.0251) 240 1.08e+0	1000 03 0		
3452 3453 3454 3455 3456	Half-Live Air: Water: Soil: Sedime	es (hr), (bas 23.3 120 240 ent: 1080	sed upon user	-entry):		
3457 3458 3459 3460	Advection Air: Water:	n Times (hr) 100 1000	:			
3461 3462 3463 3464	Sedime Level III Fu	ent: 5e+004	l (Full-Outou	t): User Koo		
3465 3466 3467 3468 3469 3470 3471 3472	Chem Name Molecular Henry's LC Vapor Pres Log Kow Soil Koc	: BBP Wt: 312.37 C: 7.61e-00 ss : 8.25e-00 : 4.73 (1 : 7.24e+00	07 atm-m3/mol 06 mm Hg (us 1ser-entered) 04 (user-ent	e (user-ente er-entered) ered)	ered)	
3473 3474 3475 3476 3476 3477 3478 3479	M Air Water Soil Sediment	lass Amount (percent) 0.0036 23.6 59.3 17	Half-Life (hr) 23.3 120 240 1.08e+0	Emissions (kg/hr) 0 1000 1000 03 0	5	

3480 3481 3482 3483 3484 3484 3485	Air Water Soil Sediment	Fugacity (atm) 1.48e-014 1.51e-012 2.7e-014 3.48e-013	Reaction (kg/hr) 0.625 796 1e+003 63.8	Advection (kg/hr) 0.21 138 0 1.99	Reaction (percent) 0.0312 39.8 50 3.19	Advection (percent) 0.0105 6.89 0 0.0995
3486 3487 3488 3489 3490 3491 3492	Persister Reaction Advectior Percent F Percent A	nce Time: 292 Time: 314 n Time: 4.1 Reacted: 93 Advected: 7	hr hr 7e+003 hr			
3493	Water Com	npartment Per	cents:			
3494 3495 3496 3497 3498 3499 3500 3501 3502 3503	Air Water water biota suspend Soil Sediment	Mass Amount (percent) 0.0036 23.6 (21.2) (0.057) ded sediment 59.3 17	Half-Life (hr) 23.3 120 (2.31) 240 1.08e+	Emission: (kg/hr) 0 1000 1000 003 0	5	
3505 3506 3507 3508 3509 3510 3511 3512 3513 3514 3515 3516	Half-Live Air: Water: Soil: Sedime Advectior Air: Water: Sedime	es (hr), (bas 23.3 120 240 ent: 1080 n Times (hr): 100 1000 ent: 5e+004	ed upon use:	r-entry):		
3517 L 3518 = 3519 3520 3521 3522 3523 3524 2525	evel III Fu Chem Name Molecular Henry's LC Vapor Pres Log Kow Soil Koc	BBP Wt: 312.37 C : 7.61e-00 SS : 8.25e-00 : 4.73 (u : 2.2e+004	(Full-Outpu ===================================	ut): EQC Defa e====== le (user-ente ser-entered) l Default)	ault ===== ered)	
3525 3526 3527 3528 3529 3530 3531 3532	Air Water Soil Sediment	lass Amount (percent) 0.00458 27.5 66 6.57	Half-Life (hr) 23.3 120 240 1.08e+	Emission: (kg/hr) 0 1000 1000 203 0	5	
3532 3533 3534 3535 3536	Air Water	Fugacity (atm) 1.69e-014 1.69e-012	Reaction (kg/hr) 0.715 832	Advection (kg/hr) 0.24 144	Reaction (percent) 0.0357 41.6	Advection (percent) 0.012 7.21

3537 3538 3539	Soil Sediment	8.86e-014 3.97e-013	1e+003 22.1	0 0.69	50 1.11	0 0.0345			
3540 3541 3542 3543 3544 3545	Persistence Time: 262 hr Reaction Time: 283 hr Advection Time: 3.62e+003 hr Percent Reacted: 92.7 Percent Advected: 7.25								
3546	Water Cor	mpartment Perc	ents:						
3547 3548 3549 3550 3551 3552 3553 2554	Air Water water biota	Mass Amount (percent) 0.00458 27.5 (26.5) (0.0712)	Half-Life (hr) 23.3 120	Emissions (kg/hr) 0 1000					
3554 3555 3556 2557	suspend Soil Sediment	ded sediment ( 66 6.57	0.875) 240 1.08e+00	1000 03 0					
3558 3559 3560 3561 3562 3563	Half-Live Air: Water Soil: Sedime	es (hr), (base 23.3 : 120 240 ent: 1080	d upon user-	entry):					
3565 3565 3566 3567 3568 3569	Advection Air: Water Sedime	n Times (hr): 100 : 1000 ent: 5e+004							