Environmental Risk Assessment of benzyl butyl phthalate (BBP)

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Risk assessment

Sources → Fate → Exposure → Toxicity

Where does it come from? Where and how is it used? Where does it end up? Does it degrade?

Are organisms exposed to it? How much?

BBP uses

- Plasticizer - used especially in PVC (vinyl flooring, foam, childrens toys)
- Adhesives
- Packaging materials
- Inks
- Arts and crafts products, paints
- Cosmetics (eg nail kits)
- Coatings for textiles
- Home maintenance (eg paint, waterproofing)
- Paint and coatings
Sources of phthalates to the environment

- Industrial production and use
- Leachate from building materials and consumer goods
- Leachate from solid waste disposal
- Leachate from litter/waste in the environment

Wastewater, run off, leachates --> freshwater and marine systems
Fate of BBP in the environment

- Water solubility 2.8 mg/L
- Log $K_{ow}$ 3.6 - 5.8
- Microbial degradation
- Photocatalytic degradation
- Half-life 1-7 days
- Low bioaccumulation
- No discernible biomagnification
BBP Mode of Action

For the medium-chain phthalates, moderate to high toxicity has been observed in numerous studies with aquatic organisms (summarized in Environment Canada, Health Canada 2015b; ECCC 2016). Results indicate that those with side-chain backbones of six or fewer carbons—i.e., DBP, BBP, DCHP, DEHP and B79P—are highly hazardous to fish, invertebrates, and algae, where LC₅₀ and effects such as behavioral abnormalities in fish, reproductive effects in daphnids, and effects on biomass in algae were observed at an exposure concentration of less than 1 mg/L. Secondary effects linked to estrogenic, thyroid-, or anti-androgenic modes of action are also relatively well documented for these substances, although inconsistent responses have been observed for alteration of VTG levels in studies with BBP and DEHP. BBP was shown to displace estradiol from the hepatic estrogen receptor, to inhibit ER binding, to either alter VTG production in rainbow trout following intra-peritoneal injection (Christiansen et al. 2000) or to have no impact on VTG levels in studies with fathead minnow (Study Submission 2014d; Harries et al. 2000), to impact gonadal histology (Study Submission...
BBP Regulatory Assessment

☑ Substance of Very High Concern (SVHC) under REACH

☑ On REACH Annex XIV (authorisation list), classified as toxic for reproduction according to Art. 57c

☑ Sunset data: 21 February 2015

☑ On REACH Annex XVII (restriction list)

Hazard classification & labelling

Danger! According to the harmonised classification and labelling (CLP00) approved by the European Union, this substance may damage the unborn child and is suspected of damaging fertility, is very toxic to aquatic life and is very toxic to aquatic life with long lasting effects.
BBP Production and Use Volumes

- In Europe: Production and import of 0-10 tons / year according to REACH dossier (1 registrant)
- Other countries: unknown

However:
- Indirect import via articles unknown
- Huge amounts embedded in infrastructure and materials at wastesites (long-term emission sources!)
Aims and Strategy

Overarching question: do the available data indicate an environmental risk?

Strategy for ecotoxicity data retrieval:
- Data compilation for US EPA’s ecotox database
- Plausibility check of the retrieved data
- Search in the primary literature
- Remove all duplicates (163 datapoints)
- Classify into „acute toxicity“ and „chronic toxicity“
- Averaging: 1 ecotoxicity estimate per species
Aims and Strategy

Overarching question: do the available data indicate an environmental risk?

Strategy for exposure data retrieval:
- Collect of all publically available monitoring data
- Delete all non-detects
- Use only data for freshwater
BBP Species-sensitivity distribution

**HC05:** Concentration that is hazardous for 5% of the species

Does **NOT** include an assessment factor.
# BBP toxicity to environmental organisms

<p>| | | |</p>
<table>
<thead>
<tr>
<th></th>
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</tr>
</thead>
<tbody>
<tr>
<td><strong>HC05</strong></td>
<td>187 nmol/L</td>
<td>Our own results</td>
</tr>
<tr>
<td><strong>Most sensitive QSAR-estimate (chronic toxicity to fish)</strong></td>
<td>300 nmol/L</td>
<td>In silico toxicity estimate</td>
</tr>
<tr>
<td><strong>PNEC (aquatic, freshwater)</strong></td>
<td>10.4 nmol/L</td>
<td>...this is the value used by ECHA</td>
</tr>
<tr>
<td><strong>Most sensitive species: Chironomus riparius</strong></td>
<td>Chronic NOECs for survival: 3.2 nmol/L</td>
<td></td>
</tr>
</tbody>
</table>
Environmental risks (Europe)
Environmental risks (North America & US)

[Graph showing concentration levels with various countries and risk levels indicated.]
Environmental risks (other countries)

- **Most sensitive species**
- **PNEC**
- **HC05**

Graph showing the relationship between concentration (nmol/L) and percentile for different countries such as China, India, Kenya, Korea, Malaysia, and South Africa.
Summary & conclusions

- BBP is found routinely in monitoring survey in the freshwater aquatic environment
- Huge differences in the amounts found
- Huge differences in the sensitivity of different organisms
- Environmental risks at highly exposed sites
BBP is found routinely in monitoring surveys in the freshwater aquatic environment. Huge differences in the amounts found. Huge differences in the sensitivity of different organisms. Environmental risks at highly exposed sites.
BBP is just one member of a big family...

Table 1-2 Subgroup 2 – Medium Chain Phthalate Esters (carbon backbone length of 3 to 7)

<table>
<thead>
<tr>
<th>CAS RN</th>
<th>Chemical Name (DSL)</th>
<th>Acronym</th>
<th>Substance Type</th>
</tr>
</thead>
<tbody>
<tr>
<td>131-16-8</td>
<td>1,2-Benzenedicarboxylic acid, dipropyl ester</td>
<td>DPrP</td>
<td>Discrete</td>
</tr>
<tr>
<td>84-68-5</td>
<td>1,2-Benzenedicarboxylic acid, bis(2-methylpropyl) ester</td>
<td>DIBP</td>
<td>Discrete</td>
</tr>
<tr>
<td>5334-09-8</td>
<td>1,2-Benzenedicarboxylic acid, cyclohexyl 2-methylpropyl ester</td>
<td>CHIBP</td>
<td>Discrete</td>
</tr>
<tr>
<td>84-64-0</td>
<td>1,2-Benzenedicarboxylic acid, butyl cyclohexyl ester</td>
<td>BCHP</td>
<td>Discrete</td>
</tr>
<tr>
<td>84-74-2</td>
<td>1,2-Benzenedicarboxylic acid, dibutyl ester</td>
<td>DBP</td>
<td>Discrete</td>
</tr>
<tr>
<td>85-65-7</td>
<td>1,2-Benzenedicarboxylic acid, butyl phenylmethyl ester</td>
<td>BBP</td>
<td>Discrete</td>
</tr>
<tr>
<td>84-61-7</td>
<td>1,2-Benzenedicarboxylic acid, dicyclohexyl ester</td>
<td>DCHP</td>
<td>Discrete</td>
</tr>
<tr>
<td>27987-25-3</td>
<td>1,2-Benzenedicarboxylic acid, bis(methylcyclohexyl) ester</td>
<td>DMCHP</td>
<td>Discrete</td>
</tr>
<tr>
<td>71868-59-6</td>
<td>1,2-Benzenedicarboxylic acid, di-C_6<del>8</del> branched alkyl esters, C_g-rich</td>
<td>DiHepP</td>
<td>Isomeric Mixture</td>
</tr>
<tr>
<td>27554-26-3</td>
<td>1,2-Benzenedicarboxylic acid, diisooctyl ester</td>
<td>DIOP</td>
<td>Isomeric Mixture</td>
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<tr>
<td>27215-22-1</td>
<td>1,2-Benzenedicarboxylic acid, isoctyl phenylmethyl ester</td>
<td>BIOP</td>
<td>Isomeric Mixture</td>
</tr>
<tr>
<td>117-51-7</td>
<td>1,2-Benzenedicarboxylic acid, bis(2-ethylhexyl) ester</td>
<td>DEHP</td>
<td>Discrete</td>
</tr>
<tr>
<td>84-75-3</td>
<td>1,2-Benzenedicarboxylic acid, dhexyl ester</td>
<td>DhHP</td>
<td>Discrete</td>
</tr>
<tr>
<td>111381-89-6</td>
<td>1,2-Benzenedicarboxylic acid, heptyl nonyl ester, branched and linear</td>
<td>79P</td>
<td>UVCB</td>
</tr>
<tr>
<td>88515-48-0; 28553-12-0</td>
<td>1,2-Benzenedicarboxylic acid, di-C_8<del>10</del> branched alkyl esters, C_9-rich; 1,2-Benzenedicarboxylic acid, diisononyl ester</td>
<td>DINP1,2</td>
<td>Isomeric Mixture</td>
</tr>
<tr>
<td>88515-40-2</td>
<td>1,2-Benzenedicarboxylic acid, benzyl C_7<del>9</del> branched and linear alkyl esters</td>
<td>B79P</td>
<td>UVCB</td>
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<tr>
<td>16883-83-3</td>
<td>1,2-Benzenedicarboxylic acid, 2,2-dimethyl-1-</td>
<td>BB4P</td>
<td>Discrete</td>
</tr>
</tbody>
</table>

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<tr>
<td>523-31-9</td>
<td>1,2-Benzenehexylic acid, bis(phenylmethyl) ester</td>
<td>DBzP</td>
<td>Discrete</td>
</tr>
</tbody>
</table>

PHTHALATES AND CUMULATIVE RISK ASSESSMENT

The Tasks Ahead

NATIONAL RESEARCH COUNCIL
Summary & conclusions

- BBP is found routinely in monitoring survey in the freshwater aquatic environment
- Huge differences in the amounts found
- Huge differences in the sensitivity of different organisms
- Environmental risks at highly exposed sites
- *What about combination effects?*

... work to be done (still)
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