Phenol & Derivatives – REACH Consortium

Qualitative Environmental Exposure Assessment

ACETOPHENONE

CAS No: 98-86-2
EINECS No: 202-708-7

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1. Environmental Exposure

1.1 General discussion

Acetophenone is released from a number of both human-made as well as natural sources.

The purpose of this chapter is to reflect qualitatively the exposure situation in the EU that results from industrial sources of acetophenone production and processing.

In the appendix predefined environmental exposure scenarios are attached to this document. These enable downstream users of acetophenone to check and reflect their specific exposure situation in regard to surface-water and soil release and to determine their conditions for a safe use as well as their acceptable use volumes. Reference is given to an according tool, that is enclosed in the registration dossier as an attached document (ECT_Acetophenone_19Jul2010.pdf) and may be downloaded from the P&D REACH Consortium-website or the web-site of the consortium members.

1.2 Production

Currently acetophenone mainly comes as a by-product of the phenol-acetone synthesis in the cumene oxidation process to cumene hydroperoxide. The cumene process is based on the Mobil-Badger process based upon a zeolite catalyst. Acetophenone is separated from heavy residues under vacuum with phenol and treated with sodium hydroxide. Then it is separated by distillation. (Clark & Macquarrie 2002).

Acetophenone's production and use as a specialty solvent for plastics and resins as well as a fragrance and flavor additive may result in its release to the environment through various waste streams (HSDB 2010).

Production sites are located in the EU (ESIS, 2010) and in the USA (HSDB 2010). Different methods of manufacturing are described:

- product from the oxidation of cumene
- oxidation of ethylbenzene
- from benzene and acetylchloride in presence of aluminum chloride
- catalytically from acetic and benzoic acids
- from benzene and acetic anhydride
- by-product in the Hock phenol synthesis

1.3 Uses

The following uses of acetophenone are described in a peer-reviewed database (HSDB 2010):

- in perfumery to impart an orange-blossom-like odor
- catalyst for the polymerization of olefins
- in organic syntheses, esp. as photosensitizer
- specialty solvent for plastics and resins

- chemical intermediate for the odorant, ethyl methyl phenylglycidate, the riot control agent, 2-chloroacetophenone, 2-bromoacetophenone for dyes, 3-nitroacetophenone, synthesis of pharmaceuticals
- flavoring agent in non-alcoholic beverages, ice cream, candy, baked goods, gelatins and puddings, chewing gum, in tobacco
- fragrance ingredient in soaps, detergents, creams, lotions, perfumes
- solvent for synthesis of pharmaceuticals, rubber, chemicals, dyestuffs and corrosion inhibitors

1.4 Natural and further releases into the environment

Natural occurrence:

Acetophenone was found in different plants like oils of *Labdanum*, *Stirlinga latifolia*, *Urtica dioica*, *Elsholtzia argyi* var. *Nipponica, Elsholtzia ciliata* in various species *of Orthodon (O. citraliferum, O. linalooliferum var. Laerolinolooliferum, O. linalooliferum, O. sabinoliferum var. Taiwanese*, in *Castoreum absolute*, and in buds of *Balsam poplar* (HSDB 2010).

Artificial Pollution Sources:

Acetophenone is a content of the heavy oil fraction of coal tar. The compound was measured in gasoline exhaust in concentrations of <0.1 to 0.4 ppm (HSDB 2010).

Furthermore, Acetophenone was identified, not quantified, in waste waters from a petrochemical plant, a propylene oxide manufacturing plant and in a surface water downstream from a tire fire location. Acetophenone has also been detected in the atmosphere from vehicular exhaust, waste incineration, residential fuel oil combustion, coal combustion, plant volatiles and vaporization of certain perfumes (HSDB 2010).

2. Environmental distribution and behaviour

2.1 Distribution

According to the available and reliable data obtained via guideline studies, the soil sorption coefficient Koc for acetophenone was determined to be in the range between 9 and 95 (Ding Y, Wang L 2000; Khan A et al. 1978; Banwart WL et al. 1980). According to the classification of Blume & Ahlsdorf, acetophenone can be regarded as a substance with very low to low binding strength to organic matter of soil and sediments.

The experimentally derived Henry's Law constants were in the range between 0.92 and 1.08 Pa m³/mol at 25°C. Based on the results of Betterton (1991), the Henry's Law constant at 20°C was calculated to be 0.766 Pa m³/mol (Staudinger J, Roberts PV 1996). The results indicate that acetophenone can be regarded as moderately volatile from aqueous solution.

Based on the physical-chemical properties the environmental distribution was calculated using Mackay Level I. According to the calculation water is by far the most important target compartment (96%) and to a minor extent air (2.9%). The other compartments were considered to be not relevant (in total ca. 1%) (Fh-ITEM 2008).

2.2 Degradation

Acetophenone introduced in water (as the main target compartment) has been shown to be **readily biodegradable** in a considerable number of reliable investigations including standard tests performed according to OECD guidelines as well as simulation tests in surface waters.

Taking into account the wide-spread natural occurrence of acetone in plants, adaptation is to be assumed in the case of microbial inocula.

The experimentally determined reaction rate constant for the reaction of acetophenone with OH radicals in the gas-phase is reported to be 2.74 x 10E-12 cm³/molecule x s. Taking into account an OH radical concentration of 5 x 10E5 radicals/cm³ (24 h day) a tropospheric half-life $t_{1/2}$ = 5.86 d can be calculated (Kwok ESC, Atkinson R 1995).

2.3 Bioaccumulation

A bioconcentration factor BCF=0.4749 was calculated using EPIWIN v3.20, BCFWIN v2.17 (Fh-ITEM 2007). Based on this result, no significant bioconcentration potential of acetophenone is to be expected.

3. Background levels

Most of the monitoring data compiled in the IUCLID (ECB, 2000) were sampled and analysed between 1970 and 2000. More recent studies dealing with the occurrence of acetophenone in the environment are scarce. Acetophenone was detected in surface waters samples collected from 139 streams (max. 0.41 µg/L, median: 0.15 µg/L; USA, 1999 -2000) (Kolpin DW et al. 2002). Furthermore, acetophenone was identified but not quantified in ground water samples at and near a landfill (USA, 2000) (Barnes KK et al. 2004). There are hints that acetophenone occurs naturally in the environment, e.g. in different plants (see section 1.4).

Unintentional releases of acetophenone into the environment were identified but the emissions were not quantified. Therefore, no background concentrations can be estimated by model calculations.

4. Ecotoxicological information

4.1 Aquatic environment

Reliable results from acute toxicity testing of three trophic levels (vertebrates, invertebrates, algae) are available; studies on long-term aquatic toxicity are not available. The most sensitive organism was found to be an alga (*Pseudokirchnerella subcapitata*: 72 h E_rC50 = 86.4 mg/L effective) (ENSR International 2003). Applying an assessment factor of 1000 according to the TGD resulted in a **PNEC aqua (freshwater) = 0.0864 mg/L**.

4.2 Terrestrial environment

There are no data available from guideline studies using sediment as test medium. In the absence of ecotoxicological data for sediment-dwelling organisms, the PNECsoil may be provisionally calculated using the equilibrium partitioning method according to ‘Guidance on information requirements and chemical safety assessment Chapter R.10 –Dose [concentration]-response regarding environment’ (ECHA 2008). With the default parameters of the TGD concerning the fractions and densities in soil as well as the substance parameters, a **PNECsoil of 0.155 mg/kg wwt** can be derived.

5. Classification for the environment

Due to its **ready biodegradablity** in the environment as well as its insignificant potential for bioaccumulation, acetophenone is not classified as dangerous/hazardous for the environment according to Directive 67/548/EEC and according to the Regulation (EC) 1272/2008 on classification, labelling and packaging of substances and mixtures (CLP Regulation):

According to Directive 67/548/EEC Annex 1 (environment): not classified

According to CLP - (EC) 1272/2008 (environment): not classified
L(E)C50 >10 - ≤100 mg/L; readily biodegradable, no bioaccumulation

Hazardous to the atmospheric environment:
(Hazardous to the ozone layer: This includes substances which are listed in Annex I to Regulation (EC) No 2037/2000 of the European Parliament and of the Council on substances that deplete the ozone layer (1) and its subsequent amendments):
Acetophenone is not listed in Annex I of (EC) No 2037/2000.

M-Factor: No
Labelling No Signal word and Pictogram for environmental hazards

6. References

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Appendix I

Predefined Emission Scenarios

Predefined emission scenarios Sheets are presented for acceptable environmental emissions in soil and surface water (PECsoil and PECsurface water).

The sheets contain maximum acceptable use volumes dependent on the local situation (e.g. ERC, dilution).

An according ECT-tool can be downloaded from the P&D REACH-Consortium web-page or the web-site of the producers. It is based on EUSES but with some simplifications to improve the user friendliness and to concentrate on the key-parameters

Predefined emission scenarios for Acetophenone (PECwater)

Use volume (t/a)	Local Release factor (%)	Removal rate (%)	dilution factor (-)	Acceptable volume (t/a)	Defined for ERC	suitable also for ERC
Default		87	10			
Site specific		87 .. 96	20 … 250			
<3	100	87	10	4,8	4 8a 8d 10 b 11b	all
<10	100	87	25	11	4 8a 8d 10 b 11b	all
<10	50	90	10	12	5	all execpt 4 8a 8d 10 11b
<10	50	90	100 (sea release)	12	5	all execpt 4 8a 8d 10 11b
<20	100	87	50	23	4 8a 8d 10 b 11b	all
<20	50	95	10	24	5	all execpt 4 8a 8d 10 11b
<20	50	95	100 (sea release)	24	5	all execpt 4 8a 8d 10 11b
<20	50	87	25	23	5	all execpt 4 8a 8d 10 11b
<50	50	87	60	57	5	all execpt 4 8a 8d 10 11b
<50	50	96	20	61	5	all execpt 4 8a 8d 10 11b
<50	6	87	100 (sea release)	79	1	all execpt 4 5 8a 8d 10b 11b
<50	6	87	10	79	1	all execpt 4 5 8a 8d 10b 11b
<100	6	87	15	119	1	all execpt 4 5 8a 8d 10b 11b
<100	6	90	100 (sea release)	103	1	all execpt 4 5 8a 8d 10b 11b
<100	6	90	10	103	1	all execpt 4 5 8a 8d 10b 11b
<100	2	87	10	238	2 6a 8b 8e	3 6d 8c 8f 10a 11a
<500	6	87	75	596	1	all execpt 4 5 8a 8d 10b 11b
<500	2	94	100 (sea release)	516	2 6a 8b 8e	3 6d 8c 8f 10a 11a
<500	1	90	100 (sea release)	619	8c 8f	3 6d 10a 11a
<500	1	87	11	524	8c 8f	3 6d 10a 11a

<1000	2	87	45	1072	8c 8f	3 6d 10a 11a
<1000	1	94	100 (sea release)	1033	8c 8f	3 6d 10a 11a
<1000	1	90	20	1239	8c 8f	3 6d 10a 11a
<1000	0,2	87	100 (sea release)	2384	3	6d 10a 11a
<5000	2	87	250	5960	8c 8f	3 6d 10a 11a
<5000	1	87	120	5722	8c 8f	3 6d 10a 11a
<5000	0,2	94	100 (sea release)	5165	3	6d 10a 11a
<5000	0,05	87	10	9537	11a	6d

Predefined Environmental Release Classes

ERC	Environmental Release Class	Default Release Fraction
ERC 1	Production of chemicals	6,00%
ERC 2	Formulation of preparations	2,00%
ERC 3	Formulation in articles	0,20%
ERC 4	Industrial use of processing aids	100,00%
ERC 5	Industrial use resulting in inclusion into or onto a matrix	50,00%
ERC 6a	Industrial use of intermediates	2,00%
ERC 6b	Industrial use of reactive processing aids	5,00%
ERC 6c	Production of plastics	5,00%
ERC 6d	Production of resins/rubbers	0,005%
ERC 7	Industrial use of substances in closed systems	5,00%
ERC 8a	Wide dispersive indoor use of processing aids in open systems	100,00%
ERC 8b	Wide dispersive indoor use of reactive substances in open systems	2,00%
ERC 8c	Wide dispersive indoor use resulting in inclusion into or onto a matrix	1,00%
ERC 8d	Wide dispersive outdoor use of processing aids in open systems	100,00%
ERC 8e	Wide dispersive outdoor use of reactive substances in open systems	2,00%
ERC 8f	Wide dispersive outdoor use resulting in inclusion into or onto a matrix	1,00%
ERC 9b	Wide dispersive outdoor use of substances in closed systems	5,00%
ERC 10a	Wide dispersive outdoor use of long-life articles and materials with low release	0,16%
ERC 10b	Wide dispersive outdoor use of long-life articles and materials with high or intended release	100,00%
ERC 11a	Wide dispersive indoor use of longlife articles and materials with low release	0,05%
ERC 11b	Wide dispersive indoor use of longlife articles and materials with high or intended release	100,00%

Predefined emission scenarios for Acetophenone (Entry route: Sludge and aereal deposition, PECsoil)

Use volume (t/a)	Local Release factor water (%)	Local Release factor air (%)	Acceptable use volume (t/a)	Defined for ERC	suitable also for ERC
<25	100	100	27,108	4 8a 8d 10 b 11b	all
<490	6	5	492	1	2 3 6a 6b 6c 8b 8e 9b 10a 11a
<1200	2	2,5	1204	2	8b 8e 10a 11a
<2500	2	0,1	2581	8b 8e	10a 11a
<25000	0,16	0,05	25817	ERC 10a	11a
<50000	0,05	0,05	54216	ERC 11a	
any	dry sludge <150 mg/kg	air release below 150 t/a	any	all	
any	dry sludge <70 mg/kg	air release below 1000 t/a	any	all	
any	dry sludge <10 mg/kg	air release below 1700 t/a	any	all	

Predefined Environmental Release Classes

ERC	Environmental Release Class
ERC 1	Production of chemicals
ERC 2	Formulation of preparations
ERC 3	Formulation in articles
ERC 4	Industrial use of processing aids
ERC 5	Industrial use resulting in inclusion into or onto a matrix
ERC 6a	Industrial use of intermediates
ERC 6b	Industrial use of reactive processing aids
ERC 6c	Production of plastics
ERC 6d	Production of resins/rubbers
ERC 7	Industrial use of substances in closed systems
ERC 8a	Wide dispersive indoor use of processing aids in open systems
ERC 8b	Wide dispersive indoor use of reactive substances in open systems
ERC 8c	Wide dispersive indoor use resulting in inclusion into or onto a matrix
ERC 8d	Wide dispersive outdoor use of processing aids in open systems
ERC 8e	Wide dispersive outdoor use of reactive substances in open systems

ERC 8f	Wide dispersive outdoor use resulting in inclusion into or onto a matrix
ERC 9a	Wide dispersive outdoor use of substances in closed systems
ERC 9b	Wide dispersive outdoor use of substances in closed systems
ERC 10a	Wide dispersive outdoor use of long-life articles and materials with low release
ERC 10b	Wide dispersive outdoor use of long-life articles and materials with high or intended release
ERC 11a	Wide dispersive indoor use of longlife articles and materials with low release
ERC 11b	Wide dispersive indoor use of longlife articles and materials with high or intended release