Substance Information Document

Acetoin

1. Substance identity

Name	Acetoin
Synonyms	3-hydroxy-2-butanone 3-hydroxybutan-2-one acetylmethylcarbinol
IUPAC Name	3-hydroxybutan-2-one
CAS	513-86-0

2. Toxicological information

Acetoin is a natural product found in Coffea arabica, Bacillus anthracis, and other organisms. It is used in the following products: perfumes and fragrances, air care products, polishes and waxes, washing & cleaning products, biocides (e.g. disinfectants, pest control products) and cosmetics and personal care products.

Acetoin is metabolized primarily via oxidation at low concentrations *in vivo* and by reduction to 2,3-butanediol at high concentrations. Production of carbon dioxide at low levels and of 2,3-butanediol at high levels is associated with the slower rate of ketone reduction (Williams, 1959). Oxidation of the terminal methyl group may result in formation of an alpha-ketoacid, which undergoes cleavage to yield carbon dioxide and a carboxylic acid fragment. Alternatively, methyl group oxidation may yield a ß-ketoacid which undergoes ß-cleavage to yield two-carbon fragments. To a minor extent, these two-carbon fragments can act as acetyl donors for acetylation of para-aminobenzoic acid (Westerfeld & Berg, 1943).

Acetoin is not acutely toxic. It has been tested in a study following OECD TG 423 (acute oral toxicity) in rats, and the resulting LD 50 is > 2000 mg/kg bw. The skin and eye irritating potential of acetoin has been evaluated in an in vitro reconstructed human epidermis model (OECD TG 439) and a bovine corneal model (OECD TG 437), respectively. The results indicated that acetoin is not irritating to skin, but it can cause irreversible damage to the eye, which leads to H318 classification under EU CLP. Two in vitro assays (OECD TG 442c and 442d) covering the two key events of the skin sensitization AOP have been performed with acetoin and the negative results indicated that it is unlikely to be a skin sensitizer. Ames test (OECD TG 471) with five *Salmonella typhimurium* strains TA97a, TA98, TA100, TA102 and TA1535 was performed to evaluate the genotoxic potential of acetoin. Based on the results of this study, it is concluded that acetoin is not mutagenic. Groups of 15 male and 15 female CFE rats were given acetoin in their drinking-water at concentrations of 0 (control), 750, 3000, or 12 000 mg/kg (equivalent to 0, 85, 330, or 1300 mg/kg bw per day (US Food & Drug Administration, 1993)). No death was observed during the study, and their condition and appearance were normal. The NOEL was set at 3000 ppm, equivalent to 330 mg/kg bw per day, based on the observed decrease in body weight, haematological changes, and increased liver weight at high dose group (Gaunt et al., 1972).

JECFA	946. Aliphatic acyclic and alicyclic a-diketones and related alpha-hydroxyketones (WHO Food Additives Series 42) (inchem.org)
FEMA	ACETOIN | FEMA (femaflavor.org)
EFSA	-
ECHA – REACH dossier	Registration Dossier - ECHA (europa.eu)
PUBCHEM	Acetoin | C4H8O2 - PubChem (nih.gov)
CIR	-
OSHA	ACETOIN | Occupational Safety and Health Administration (osha.gov)

3. Addictiveness and attractiveness

No substance specific data were identified.

SCENIHR	-
EMA	-
PUBMED	-

Reference

- Williams, T.R. (1959) Detoxication Mechanisms: The Metabolism and Detoxication of Drugs, Toxic Substances and Other Organic Compounds, 2nd Ed., London, Chapman & Hall, pp. 62, 78.
- Westerfeld, W.W. & Berg, R.L. (1943) Observations on the metabolism of acetoin. J. Biol. Chem., 148, 523-528.
- Gaunt, I.F., Branton, P.G., Kiss, I.S., Grasso, P. & Gangolli, S.D. (1972) Short-term toxicity of acetoin (acetyl methylcarbinol) in rats. Food Cosmet. Toxicol., 10, 131-141.