# Substance Information Document

Isobutyric acid

## 1. Substance identity

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| Name | Isobutyric acid |
| Synonyms | 2-methylpropanoic acid; 2-Isopropylcyclohexanol; 2-Methylpropionic acid; Acetic acid, dimethyl-; Dimethylacetic acid; Isobutanoic acid; Isobutyric acid (natural); Isopropylformic acid; Propanoic acid, 2-methyl-; Propionic acid, 2-methyl-; Alpha-Methylpropanoic acid |
| IUPAC Name | 2-methylpropanoic acid |
| CAS | 79-31-2 |

## 2. Toxicological information

The acute oral and dermal $LD_{50}$ values for isobutyric acid are >500 mg/kg/bw (rat) and >200 mg/kg/bw (rabbit), respectively. Data are available for the anhydride via the inhalation route indicating a low toxicity with an $LC_{50}$ value of >5.1 mg/L. Both the acid and anhydride forms are considered moderate to severe eye irritants. Isobutyric acid is a moderate to severe skin irritant and is corrosive to skin. Based on clinical signs observed in the $LC_{50}$ study (e.g. rales, nasal secretions, weight loss) airborne isobutyric acid or isobutyric anhydride can cause irritation of the upper respiratory tract.

Repeated inhalation exposures would likely exacerbate the irritative effects. Although reported as a non-sensitizer, sensitization data are not available.

Repeated exposures to moderate to high concentrations of isobutanol (the metabolic precursor of isobutyric acid) are well tolerated in rats as observed in a 90-day inhalation study where rats were exposed to isobutanol up to 2500 ppm. Based on these findings, the NOAEC for repeated dose toxicity is considered to be 2500 ppm (ca. 7700 mg/m³) for males and females. In a 13-week oral gavage study, conducted with isobutanol up to 1000 mg/kg, a NOAEL of 316 mg/kg bw/day has been observed.

An inhalation two-generation reproductive toxicity study conducted with isobutanol (up to 2500 ppm) did not cause any parental systemic, reproductive, or neonatal toxicity when administered for two generations via whole-body exposure. No adverse developmental effects were noted in rats or rabbits exposed to 10 mg/L isobutanol during gestation.

Based on *in vitro* studies, isobutyric acid is not mutagenic in bacteria and mammalian cells and no evidence of genotoxicity was observed in an *in vivo* mouse micronucleus test conducted with isobutanol administered once orally to male and female NMRI mice at doses up to 2000 mg/kg body weight.

No substance specific data were identified for carcinogenicity.

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| JECFA | No safety concern at current levels of intake when used as a flavouring agent.<br>907. Saturated aliphatic acyclic branched-chain primary alcohols, aldehydes/acids (WHO Food Additives Series 40) (inchem.org) |
| FEMA | - |
| EFSA | - |
| ECHA – REACH dossier | Registration Dossier - ECHA (europa.eu) |
| PUBCHEM | Isobutyric acid \| C4H8O2 - PubChem (nih.gov) |
| CIR | - |
| OSHA | - |

## 3. Addictiveness and attractiveness

No substance specific data were identified.

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| SCENIHR | - |
| EMA | - |
| PUBMED | - |