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# 2-Butanethiol

## MAK Value Documentation – Translation of the German version from 2021

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**Keywords**

2-butanethiol; haematotoxicity; olfactory epithelium; irritation; skin absorption; toxicity; maximum workplace concentration; MAK value

## Abstract

The German Commission for the Investigation of Health Hazards of Chemical Compounds in the Work Area has evaluated data for 2-butanethiol [513-53-1] considering all toxicological end points. Data from a 90-day inhalation study with rats show that the critical effects are haematotoxicity and histopathological alterations in the nasal olfactory epithelium. On the basis of the NOAEC of 25 ml/m$^3$ for systemic toxicity and taking into account the increased respiratory volume at the workplace, the maximum concentration at the workplace (MAK value) has been set at 2 ml/m$^3$. Local effects in the nose can be ruled out at this concentration. As the critical effect is systemic, Peak Limitation Category II has been assigned with an excursion factor of 2. As data for developmental toxicity are not available, 2-butanethiol has been classified in Pregnancy Risk Group D. According to skin absorption models, percutaneous absorption is expected to contribute significantly to systemic toxicity. Therefore, 2-butanethiol has been designated with an "H". No studies of the sensitizing, genotoxic or carcinogenic potential of the substance are available.

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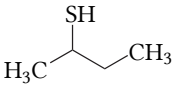
| | |
|---|---|
| **MAK value (2020)** | **2 ml/m³ (ppm) ≙ 7.5 mg/m³ [a)]** |
| **Peak limitation (2020)** | **Category II, excursion factor 2** |
| **Absorption through the skin (2020)** | **H** |
| **Sensitization** | – |
| **Carcinogenicity** | – |
| **Prenatal toxicity (2020)** | **Pregnancy Risk Group D** |
| **Germ cell mutagenicity** | – |
| **BAT value** | – |
| Synonyms | *sec*-butanethiol<br>*sec*-butyl mercaptan<br>1-methyl-1-propanethiol |
| Chemical name (IUPAC) | butane-2-thiol |
| CAS number | 513-53-1 |
| Structural formula |  |
| Molecular formula | $C_4H_{10}S$ |
| Molar mass | 90.18 g/mol |
| Melting point | −165 °C (NLM 2020) |
| Boiling point at 1013 hPa | 84.5 °C (NLM 2020) |
| Density at 17 °C | 0.83 g/cm³ (NCBI 2022) |
| Vapour pressure at 25 °C | 108 hPa (NLM 2020) |
| log $K_{OW}$ | 2.18 (calculated; NLM 2020) |
| Solubility | 1.32 g/l water (NLM 2020) |
| **1 ml/m³ (ppm) ≙ 3.742 mg/m³** | **1 mg/m³ ≙ 0.267 ml/m³ (ppm)** |

[a)] Even if the MAK value is observed, "odour-associated" symptoms cannot be ruled out in individual cases.

2-Butanethiol is added to odourless gases as a warning substance, it is used as an industrial solvent and occurs as an intermediate of insecticides and herbicides (Kim et al. 2009). In the EU, 2-butanethiol is an approved food additive (European Commission 2012). The substance has a stereocentre; the CAS number for the (*R*)-form is 52945-73-0 and that for the (*S*)-form 20407-74-3. Unless otherwise stated in the studies, it is assumed that the racemate was used.

# 1 Toxic Effects and Mode of Action

After inhalation exposure for 90 days, haemosiderosis of the spleen and effects in the olfactory epithelium were observed in rats at about 100 ml/m³ and above.

There are no data available for fertility, developmental toxicity, genotoxicity, carcinogenicity or sensitization.

## 2 Mechanism of Action

As was already described in the documentation for 1-butanethiol from 2000 (Greim 2005), thiols can contribute to the formation of reactive oxygen species through autoxidation in the presence of suitable metal ions. The resulting disulfides are reduced again to thiols. This redox cycling leads to oxidative stress. The haemolytic effect typical of aliphatic thiols can be seen, among other things, in the formation of Heinz bodies (clumping of irreversibly denatured haemoglobin). As a result, the number of erythrocytes decreases as they lose their deformability and are destroyed in the reticulohistiocytic system. Erythroclasia occurs mainly in the spleen, recognizable by its enlargement and dark discoloration. A decrease in circulating erythrocytes stimulates compensatory erythropoiesis, but anaemia occurs if there is too little new formation (Munday 1989). This effect can be assumed also for 2-butanethiol and is confirmed by the findings in the spleen and a reduced erythrocyte count from the studies in rats with repeated inhalation exposure (see Section 5.2.1).

The bioactivity of 2-butanethiol was investigated in 398 in vitro assays during the US EPA's ToxCast/Tox21 testing programme and the results were negative in all of them (US EPA 2020).

Thiols have a very high affinity to olfactory receptors (Li et al. 2016). Therefore, their odour threshold is very low and due to the sulfur content in these molecules, the odour quality is very similar to that of hydrogen sulfide, which smells like rotten eggs (Schiffman and Williams 2005). For this reason, these chemicals are added to odourless gases as odorants. This takes advantage of the biological function of such odours, which is based primarily on hazard prevention (Stevenson 2010). This association is learned (Hatt 2019), and therefore individuals from different cultures sometimes react very differently to odours (Ayabe-Kanamura et al. 1998).

Some substances can directly trigger "odour-associated" symptoms such as nausea or headaches in some individuals. There is generally no information in the scientific literature about the physiological mechanisms that trigger these symptoms, but it is mainly very odour-intensive substances that can cause such reactions in individual cases (DFG 2021).

## 3 Toxicokinetics and Metabolism

On the basis of toxicity studies in animals, absorption via the respiratory and gastrointestinal tract can be assumed. However, quantitative data are not available.

According to the formula of Buist et al. (2012), the blood:air partition coefficient of 2-butanethiol is 14.

Calculations based on the IH SkinPerm model (Tibaldi et al. 2014) and according to the algorithm of Fiserova-Bergerova et al. (1990) yield dermal penetration rates of 0.033 and 0.482 mg/cm$^2$ and hour, respectively, for a saturated aqueous solution. Exposure of both hands and forearms (2000 cm$^2$ of skin) for 1 hour would thus result in absorbed amounts of 66 and 964 mg, respectively.

Several metabolic pathways are known for simple thiols in mammals: *S*-methylation leads to the formation of a methyl thioether or sulfide with subsequent oxidation to the corresponding sulfoxides and sulfones. Furthermore, thiols can react with glutathione and form mixed disulfides. Especially in the case of thiols with a low molar mass, oxidative desulfurization can take place with the formation of carbon dioxide and sulfate (WHO 2000). These metabolic pathways are assumed also for 2-butanethiol.

## 4 Effects in Humans

No data are available for the end points of single and repeated exposures, reproductive toxicity, genotoxicity, carcinogenicity or for allergenic effects of 2-butanethiol.

Humans can smell 2-butanethiol concentrations as low as 10 µl/m$^3$ (no other details; Kim et al. 2009).

The most common effects after exposure to thiols are headaches and nausea, triggered by the strong and annoying odour. High concentrations may cause unconsciousness accompanied by cyanosis, a cold sensation of the extremities, acceleration of the pulse or pulmonary oedema (no other details; Kim et al. 2009).

In a volunteer study with **2-methyl-2-propanethiol** (IIT Research Institute 1982; see Hartwig and MAK Commission 2023), it was shown that the substance can be perceived very well by the sense of smell. 2-Methyl-2-propanethiol triggers unpleasant sensations, but all test persons exhibited adaptation to the odour, which in some cases was rapid. This is to be expected also for 2-butanethiol.

However, it must be noted that the volunteer study with 2-methyl-2-propanethiol was carried out with considerably lower concentrations in relation to its MAK value of up to a maximum of 65 µl/m$^3$ (which is only 6.5% of the MAK value for 2-methyl-2-propanethiol). Generally, adaptation to an odour is based on the calcium-dependent regulation of the responsiveness of the cAMP-gated ion channels (CNG channels). Activation of the olfactory receptors by an odorant leads to an increase in the cAMP concentration in the nerve cell, which triggers the opening of these CNG channels and allows $Ca^{2+}$ ions to flow into the cell. This leads to the action potential and thus to the perception of odour in the brain. The $Ca^{2+}$ ions flowing into the olfactory sensory cell through the CNG channels bind intracellularly to calmodulin, which in turn blocks the further influx of $Ca^{2+}$ ions, so that odour perception decreases despite constant activation of the olfactory receptors by the odorant (Hatt 2019). In principle, this mechanism is to be expected also for higher concentrations.

# 5 Animal Experiments and in vitro Studies

## 5.1 Acute toxicity

### 5.1.1 Inhalation

There are no data available.

### 5.1.2 Oral administration

The oral $LD_{50}$ of 2-butanethiol in the rat is 5176 mg/kg body weight, which is much higher than that for 1-butanethiol (1500 mg/kg body weight). The animals exhibited ataxia and loss of body weight (no other details; Farr and Kirwin 1994).

### 5.1.3 Dermal application

The dermal $LD_{50}$ in the rat is greater than 2000 mg/kg body weight (Farr and Kirwin 1994).

## 5.2 Subacute, subchronic and chronic toxicity

### 5.2.1 Inhalation

In a 90-day inhalation study carried out according to OECD Test Guideline 413, groups of 10 male and 10 female Sprague Dawley rats were exposed whole-body to 2-butanethiol concentrations of 0, 25, 99 or 400 ml/m$^3$ for 6 hours daily, on 5 days per week. After exposure to 99 ml/m$^3$, haemosiderin accumulation in the spleen (3/10; controls: 0/10) and eosinophilic inclusions in the nasal turbinates (2/10; controls: 0/10) were observed in the males, reaching statistical significance only at the high concentration. Another target organ is the kidney, where hyaline droplets in the tubules, granular inclusions, pyelonephritis and tubular degeneration or regeneration were observed in the males of the 400 ml/m$^3$ group; the females likewise exhibited pyelonephritis (Kim et al. 2009). Thus, the effects already occurred at 99 ml/m$^3$, so that the NOAEC (no observed adverse effect concentration) for systemic and local effects in this study was

25 ml/m³ and not, as the authors stated, 99 ml/m³. The changes in the noses of the animals are interpreted as the result of the irritant effect of 2-butanethiol (Table 1).

**Tab. 1** 90-day inhalation study with 2-butanethiol in rats

| Species, strain, number per group | Exposure | Findings | Reference |
|---|---|---|---|
| **rat**, Sprague Dawley, 10 ♂, 10 ♀ | **90 days**, 0, 25, 99, 400 ml/m³, 6 hours/day, 5 days/week, **OECD Test Guideline 413** | **25 ml/m³**: **NOAEC** (local and systemic), no abnormal behaviour (odour); **99 ml/m³**: ♂: spleen (haemosiderin accumulation; 3/10, not statistically significant), olfactory epithelium (eosinophilic inclusions 2/10, not statistically significant); **400 ml/m³**: ♂, ♀: food consumption ↓, erythrocytes ↓, haemoglobin ↓, haematocrit ↓, relative kidney weights ↑, ALT ↓; ♂: relative liver weights (19%) ↑, histopathological effects in the kidneys (hyaline droplets in the tubules, granular inclusions, pyelonephritis, tubular degeneration/regeneration), spleen (haemosiderin accumulation, 10/10), liver (centrilobular hypertrophy of the hepatocytes, 2/10, not statistically significant), olfactory epithelium (eosinophilic inclusions 6/10[a]); mineralization, 3/10, not statistically significant); ♀: body weight development ↓, relative weights of brain, lungs, heart ↑; MCV ↑, MCHC ↓, pyelonephritis (5/10; not statistically significant) | Kim et al. 2009 |

[a] calculated retrospectively with Fisher's exact test: $p < 0.05$
ALT: alanine aminotransferase; MCHC: mean corpuscular haemoglobin concentration; MCV: mean corpuscular volume

### 5.2.2 Oral administration

There are no data available.

### 5.2.3 Dermal application

There are no data available.

## 5.3 Local effects on skin and mucous membranes

Application of 2-butanethiol to the skin of rabbits for 4 hours did not cause any skin reactions (no other details; Farr and Kirwin 1994).

The instillation of 2-butanethiol into one eye in rabbits caused acute pain reactions and moderate conjunctival irritation, which lasted for 2 days. There was also mild irritation of the iris, which regressed after 1 day (no other details; Farr and Kirwin 1994).

## 5.4 Allergenic effects

No data are available for the sensitizing potential of 2-butanethiol. However, the positive findings in the local lymph node assay with two structurally very closely related substances, 1-butanethiol and 2-methyl-2-propanethiol (Hartwig and MAK Commission 2020, 2023), make a contact sensitizing potential seem likely also for 2-butanethiol.

## 5.5 Reproductive and developmental toxicity

There are no data available.

## 5.6 Genotoxicity

There are no data available.

### 5.7 Carcinogenicity

There are no data available.

## 6 Manifesto (MAK value/classification)

The critical effects of 2-butanethiol are effects on erythrocytes, the spleen and the olfactory epithelium of the nose, and mucosal irritation.

**MAK value.** Data in humans that would allow the derivation of a MAK value are not available. As with all thiols, 2-butanethiol is a substance with a strong, unpleasant odour. Humans can smell 2-butanethiol concentrations as low as 10 µl/m$^3$ (no other details; Kim et al. 2009).

For 2-butanethiol, a 90-day inhalation study in rats is available, in which the local and systemic NOAEC was 25 ml/m$^3$ (Kim et al. 2009). At the next-higher concentration of 99 ml/m$^3$ haemosiderosis in the spleen and local effects in the olfactory epithelium were observed. The derivation of a MAK value for a local and for a systemic effect differs. Thus, based on the systemic effect and the NOAEC of 25 ml/m$^3$, the extrapolation of the data from animal experiments to humans (1:2), taking into account the increased respiratory volume of humans at the workplace compared with that of test animals at rest (1:2) and assuming a possible increase in effects with chronic exposure (1:2), a concentration of 3.13 ml/m$^3$ is calculated. Using the preferred value approach, the MAK value is 2 ml/m$^3$. Based on the NOAEC of 25 ml/m$^3$ for local effects, the application of the procedure presented in Brüning et al. (2014) results in a concentration of 6.25 ml/m$^3$ for locally irritant substances, taking into account the expected increase in effects with chronic exposure. Using the preferred value approach, the MAK value would be 5 ml/m$^3$. Thus, a MAK value of 2 ml/m$^3$ has been derived for 2-butanethiol on the basis of the systemic effect, which also protects against the local effects.

Similar systemic effects were observed in several studies with inhalation exposure of rats to 2-butanethiol, 2-methyl-2-propanethiol and 1-butanethiol. The limit values derived from these studies are of the same order of magnitude and are lower than the limit values that would be derived on the basis of local effects (Hartwig and MAK Commission 2020, 2023).

Not only are acute annoyance reactions or disgust triggered by odours, but some individuals may also experience "odour-associated" symptoms such as headaches or nausea (no other details regarding thiols; Shusterman 1999). However, respective studies with 2-butanethiol are not available. Therefore, it cannot be ruled out that 2-butanethiol causes reversible "odour-associated" symptoms even if the MAK value of 2 ml/m$^3$ is observed. Pathophysiological mechanisms for these symptoms are not described in the scientific literature. For comparison, after 3 hours of daily exposure (for 5 or 10 days) of subjects (n = 2 and n = 1, respectively) to ethanethiol, irritation of the oral and nasal mucous membranes, nausea and changes in the sense of taste occurred at the concentration of 3.9 ml/m$^3$, but not at 0.39 ml/m$^3$ (Blinova 1965).

**Peak limitation.** Since the MAK value for 2-butanethiol is derived on the basis of the systemic effect, the substance has been assigned to Peak Limitation Category II. Information on the half-life of the substance is not available. Therefore, the excursion factor has been established at the default level of 2 for substances with systemic effects. Thus, the permissible short-term concentration is also below the locally effective concentration.

**Prenatal toxicity.** Since no developmental toxicity data are available for 2-butanethiol and the MAK value of 2 ml/m$^3$ is twice as high as the MAK values of 1-butanethiol and 2-methyl-2-propanethiol, which are both assigned to Pregnancy Risk Group C, 2-butanethiol has been assigned to Pregnancy Risk Group D.

**Absorption through the skin.** The acute toxicity of 2-butanethiol after dermal application is low. Apart from this, no experimental data are available to assess absorption through the skin. Calculations based on models yielded dermally absorbed amounts of 66 and 964 mg under standard conditions (1 hour, 2000 cm$^2$ of skin) (Section 3). An 8-hour exposure (10 m$^3$ respiratory volume) at the level of the MAK value, assuming complete absorption, would correspond to an

absorbed amount of 74.8 mg of 2-butanethiol via the respiratory tract. Thus, dermal exposure may result in systemic toxicity even if the MAK value is observed. Therefore, 2-butanethiol has been designated with an "H" (for substances which can be absorbed through the skin in toxicologically relevant amounts).

**Sensitization.** There are no data available for the sensitizing effects of 2-butanethiol. The positive findings in valid local lymph node assays with two structurally very closely related substances, namely 1-butanethiol and 2-methyl-2-propanethiol (Hartwig and MAK Commission 2020, 2023), suggest contact sensitizing potential also for 2-butanethiol, but since no positive results are available for 2-butanethiol itself, the substance has not been designated with "Sh" or "Sa" (for substances which cause sensitization of the skin or airways).

**Germ cell mutagenicity and carcinogenicity.** Studies of the genotoxicity and carcinogenicity of the substance are not available. Based on the structure and the data for structurally similar thiols, genotoxic or carcinogenic effects are not to be expected. 2-Butanethiol has therefore not been classified in one of the categories for germ cell mutagens or carcinogens.

# Notes

### Competing interests

The established rules and measures of the commission to avoid conflicts of interest (www.dfg.de/mak/conflicts_interest) ensure that the content and conclusions of the publication are strictly science-based.

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