| Compound | n-Butanal, n-Butyraldehyde | | Data collection sheet |
|---|---|---|---|
| **N°CAS** 123-72-8 | **EU- Classification:** Not classified<br>**CLP:** Acute Tox., Skin Irrit., Eye Irrit., Asp. Tox. | | |
| | | | |
| **Organization Name** | | | |
| **Risk Value Name** | LOAEC | NOAEC | LOAEC |
| **Risk Value (mg/m³)** | **363** | **145** | **360** |
| **Risk Value (ppm)** | 125 | 50 | 125 |
| **Reference period** | Subchronic | Subchronic | Subchronic |
| **Year** | 1979 | 1980 | 1979 |
| **Key Study** | Union Carbide Corporation, 1979 OECS-SIDS 2005 | Union Carbide Corporation, 1980 OECS-SIDS 2005 | Union Carbide Corporation, 1979 OECS-SIDS 2005 |
| **Study type** | Subchronic | Subchronic | Subchronic |
| **Species** | F 344 rats | rats | |
| **Duration of exposure in pivotal study** | 6h/day, 5 days/week, 13 weeks | 6h/day, 5 days/12 weeks | 6h/day, 5 days/week, 14 weeks |
| **Critical effect** | Squamous metaplasia of the nasal cavity | | Goblet cell hyperplasia within the nasal mucosa |
| **Critical dose value** | | | |
| **Adjusted critical dose** | | | |
| **Single assessment factors (see table R.8.6)** | | | |
| **Other effects** | | | |

| Compound | n-Butanal (n-Butyraldehyde) | | Factsheet |
|---|---|---|---|
| **Parameter** | **Note** | **Comments** | **Value / descriptor** |
| **EU-LCI Value and Status** | | | |
| EU-LCI value | 1 | Mass/volume [µg/m³] | 650 |
| EU-LCI status | 2 | Draft / Final | Final |
| EU-LCI year of issue | 3 | Year when the EU-LCI value has been issued | 2013 |
| **General Information** | | | |
| CLP-INDEX-Nr. | 4 | INDEX | 605-006-00-2 |
| EC-Nr. | 5 | EINECS – ELINCS - NLP | 204-646-6 |
| CAS-Nr. | 6 | Chemical Abstract Service number | 123-72-8 |
| Harmonised CLP classification | 7 | Human Health Risk related classification | not harmonized |
| Molar mass | 8 | [g/mol] | 72.11 |

| **Key Data / Database** | | | |
|---|---|---|---|
| Key study, Author(s), Year | 9 | Critical study with lowest relevant effect level | Union Carbide 1980, OECD SIDS (2005) |
| Read across compound | 10 | Where applicable | |
| Species | 11 | rat,… human | Rat |
| Route/type of study | 12 | Inhalation, oral feed, … | Inhalation |
| Study length | 13 | Days, subchronic, chronic | Subchronic |
| Exposure duration | 14 | Hrs/day, days/week | 6/24;5/7d; 13 wks |
| Critical endpoint | 15 | Effect(s), site of | Irritation (squamous metaplasia of the nasal cavity) |
| Point of departure (POD) | 16 | LOAEC*L, NOAEC*L, NOEC*L, Benchmark dose, …. | NOAEC |
| POD Value | 17 | [mg/m$^3$] or [ppm] | 145 mg/m$^3$ and 50 ppm |
| **Assessment Factors (AF)** | **18** | | |
| Adjustment for exposure duration | 19 | Study exposure hrs/day, days/week | 5.6 |
| AF Study Length | 20 | sa→ sc→ c *(R8-5)* | 2 |
| Route-to-route extrapolation factor | 21 | | |
| AF Dose-response | 22 a | Reliability of dose-response, LOAEL → NOAEL | |
| | 22 b | Severity of effect *(R 8-6d)* | |
| Interspecies differences | 23 a | Allometric Metabolic rate *(R8-3)* | |
| | 23 b | Kinetic + dynamic | |
| Intraspecies differences | 24 | Kinetic + dynamic Worker - General population | 10 |
| AF (sensitive population) | 25 | Children or other sensitive groups | |
| Other adjustment factors Quality of whole database | 26 | Completeness and consistency Reliability of alternative data *(R8-6 d,e)* | 2 |
| **Result** | | | |
| Summary of assessment factors | 27 | Total Assessment Factor (TAF) | 224 |
| POD/TAF | 28 | Calculated value (µg/m$^3$ and ppb) | 662.1 µg/m$^3$ 223.2 ppb |
| Molar adjustment factor | 29 | Used in read-across | |
| Rounded value | 30 | [µg/m$^3$] | 650 |
| **Additional Comments** | 31 | | |
| | | | |
| **Rationale Section** | 32 | | |

In a non verifiable repeated-dose inhalation study male and female F344 rats were exposed by inhalation to n-butyraldehyde vapor at concentrations of 0, 125, 500, or 2000 ppm (0, 363, 1450, or 5800 mg/m$^3$) for 6 hr/day, 5 days per week, for 13 weeks (Union Carbide Corporation, 1979). Animals in all treatment groups displayed a significant increase in the incidence of squamous metaplasia of the nasal cavity. This study resulted in a LOAEC of 125 ppm.

A subsequent 12-week inhalation study in male and female rats employing lower doses of 0, 1, 10, and 50 ppm (145 mg/m$^3$) n-butyraldehyde did not result in any adverse effects on the nasal, olfactory, or respiratory epithelial tissues resulting in a NOAEC of 50 ppm (Union Carbide Corporation, 1980).

In another study, beagle dogs were exposed by inhalation to n-butyraldehyde vapor at concentrations of 0, 125, 500, and 2000 ppm for 6 hr/day, five days a week, for 14 weeks. Dogs exposed to 125 and 500 ppm displayed goblet cell hyperplasia within the nasal mucosa (Union Carbide Corporation, 1979).

The NOAEC of 50ppm (145 mg/m$^3$) from the rat-study is used for derivation of a LCI. The subchronic NOAEC is divided by standard factors for study duration (2) and exposure duration (5.6). Rat and dogs -compared to humans –are considered equally sensitive. Thus no interspecies factor is used. For interspecies variation a factor of 10 is used. With the quality of the data base considered as insufficient a factor of 2 is selected.

The EU-LCI is above the odour detection threshold of ~2 µg/m$^3$ (Cometto-Muniz 2010).

**References**

OECS SIDS (2005) N-Valeraldehyde. UNEP Publications. Washington.

Ernstgard L, Iregren A, Sjögren B et al. (2006) Acute effects of exposure to hexanal vapors in humans. J Occup Environ Med 48: 573-580.

Cometto-Muniz JE, Abraham MH (2010) Odor detection by humans of lineal aliphatic aldehydes and helional as gauged by dose-response functions. Chem Senses 35:289-299.