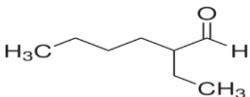
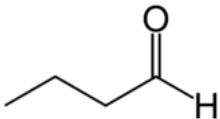


| Compound | 2-Ethyl hexanal (read-across from n-Butanal) | | Factsheet |
|-------------------------------------|---|--|-------------------------|
| Parameter | Note | Comments | Value / descriptor |
| EU-LCI Value and Status | | | |
| EU-LCI value | 1 | Mass/volume [$\mu\text{g}/\text{m}^3$] | 900 |
| 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 | |
| EC-Nr. | 5 | EINECS – ELINCS – NLP | 204-596-5 |
| CAS-Nr. | 6 | Chemical Abstract Service number | 123-05-07 |
| Harmonised CLP classification | 7 | Human Health Risk related classification | Not harmonized |
| Molar mass | 8 | [g/mol] | 128.21 |
| Key Data / Database | | | |
| Key study, Author(s), Year | 9 | Critical study with lowest relevant effect level | |
| Read across compound | 10 | Where applicable | n-Butanal |
| Species | 11 | rat,... human | |
| Route/type of study | 12 | Inhalation, oral feed, ... | |
| Study length | 13 | Days, subchronic, chronic | |
| Exposure duration | 14 | Hrs/day, days/week | |
| Critical endpoint | 15 | Effect(s), site of | |
| Point of departure (POD) | 16 | LOAEC*L, NOAEC*L, NOEC*L, Benchmark dose, | EU-LCI for n-Butanal |
| POD Value | 17 | [mg/m ³] or [ppm] | 0.662 mg/m ³ |
| Assessment Factors (AF) | | | |
| Adjustment for exposure duration | 19 | Study exposure hrs/day, days/week | |
| AF Study Length | 20 | sa → sc → c (R8-5) | |
| 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 | |
| AF (sensitive population) | 25 | Children or other sensitive groups | |
| Other adjustment factors | 26 | Completeness and consistency | |
| Quality of whole database | | Reliability of alternative data (R8-6 d,e) | |

| | | | |
|-------------------------------|----|---|------|
| Result | | | |
| Summary of assessment factors | 27 | Total Assessment Factor (TAF) | |
| POD/TAF | 28 | Calculated value ($\mu\text{g}/\text{m}^3$ <u>and</u> ppb) | |
| Molar adjustment factor | 29 | Used in read-across (100.16/72.11) | 1.39 |
| Rounded value | 30 | $[\mu\text{g}/\text{m}^3]$ ($6.1 \mu\text{g}/\text{m}^3 \times 1.39 = 920.3 \mu\text{g}/\text{m}^3$) | 900 |
| Additional Comments | 31 | | |
| | | | |
| Rationale Section | 32 | | |

Rationale for read-across

- Data poor compound: no adequate toxicological data for 2-ethyl hexanal exist from which a LCI could be derived directly using the de novo procedure.
- Read-across from EU-LCI value of butanal: within the chemical class 'saturated aldehydes', butanal is the closest homologue compound with an EU-LCI value: two additional CH_2 group in the aliphatic main side chain of 2-ethyl hexanal, and one in the second minor side chain.
- Toxicological critical endpoint for butanal: irritation (squamous metaplasia of the nasal cavity).
- The key assumption underlying the read across of the EU-LCI value from butanal to 2-ethyl hexanal is that both compounds have the same critical endpoint (irritation) and this is caused by the common functional group (and not by the additional CH_2 groups).

| Compound | Structure | MW [g/mol] | EU-LCI value |
|-----------------|---|---------------|---|
| 2-ethyl hexanal |  | 128.21 | ? (read-across to be used) $900 \mu\text{g}/\text{m}^3$ |
| butanal |  | 72.11 | $650 \mu\text{g}/\text{m}^3$ (de novo protocol) Unrounded value: $662.1 \mu\text{g}/\text{m}^3$ or 223.2 ppb |

- Unrounded EU-LCI value of butanal: $662.1 \mu\text{g}/\text{m}^3 \rightarrow$ to be used for read across EU-LCI of 2-ethyl hexanal.
- Cut-off rule in place: difference in chain length between the two homologue compounds is larger than two CH_2 groups per aliphatic chain \rightarrow cut-off to hexanal.
- Thus, EU-LCI value for 2-ethyl hexanal is $662.1 \mu\text{g}/\text{m}^3$. After MW conversion at 23 °C and 1.013 atm (+ cut-off rule at 2C): EU-LCI 2-ethyl hexanal = $662.1 \mu\text{g}/\text{m}^3 \times 1.39 = 920.3 \mu\text{g}/\text{m}^3 \rightarrow$ rounded to $900 \mu\text{g}/\text{m}^3$.