

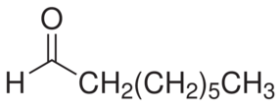
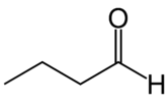
Compound	n-Octanal (read-across from n-Butanal)		Factsheet
Parameter	Note	Comments	Value / descriptor
EU-LCI Value and Status			
EU-LCI value	1	Mass/volume [$\mu\text{g}/\text{m}^3$]	900
EU-LCI status	2	Draft / Final	Final
EU-LCI year of issue	3	Year when the EU-LCI value has been issued	2013
General Information			
CLP-INDEX-Nr.	4	INDEX	
EC-Nr.	5	EINECS – ELINCS – NLP	
CAS-Nr.	6	Chemical Abstract Service number	124-13-0
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 Quality of whole database	26	Completeness and consistency 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)	1.39
Rounded value	30	$[\mu\text{g}/\text{m}^3]$	900
Additional Comments	31		

Rationale Section

Rationale for read across

- Data poor compound: no adequate toxicological data for octanal 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: four additional CH₂ group in the aliphatic side chain of octanal.
- 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 octanal is that both compounds have the same critical endpoint (irritation) and this is caused by the common functional group (and not by the additional CH₂ group).

Compound	Structure	MW [g/mol]	EU-LCI value
octanal		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 for butanal: 662.1 $\mu\text{g}/\text{m}^3$ → to be used for read-across EU-LCI of octanal.
- Cut-off rule in place: difference in chain length between the two homologue compounds is larger than two CH₂ groups per aliphatic chain → cut-off to hexanal.
- Thus, EU-LCI value for octanal 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 octanal = 662.1 $\mu\text{g}/\text{m}^3$ x 1.39 = 920.3 $\mu\text{g}/\text{m}^3$ → rounded to 900 $\mu\text{g}/\text{m}^3$.
- The EU-LCI is above the odour detection threshold of ~ 2 $\mu\text{g}/\text{m}^3$ (Cometto-Muniz 2010).

References

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.