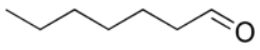
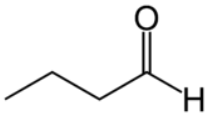
Compound	**n-Heptanal (read-across from n-Butanal)**		**Factsheet**
Parameter	**Note**	**Comments**	**Value / descriptor**
EU-LCI Value and Status			
EU-LCI value	1	Mass/volume [µg/m^3]	900
EU-LCI status	2	Draft / Final	Final
EU-LCI year of issue	3	Year when the EU-LCI value has been issued	2013
General Information			
CLP-INDEX-Nr.	4	INDEX	
EC-Nr.	5	EINECS – ELINCS – NLP	203-898-4
CAS-Nr.	6	Chemical Abstract Service number	111-71-7
Harmonised CLP classification	7	Human Health Risk related classification	Not harmonized
Molar mass	8	[g/mol]	114.18
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)	**18**		
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 (µg/m³ and ppb)	
Molar adjustment factor	29	Used in read-across (100.16/72)	1.39
Rounded value	30	[µg/m³]	900
Additional Comments	31		
Rationale Section	32		

Rationale for read across

- Data poor compound: no adequate toxicological data for heptanal 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: three additional CH2 group in the aliphatic side chain of heptanal.
- 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 heptanal 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 group).

Compound	Structure	MW [g/mol]	EU-LCI value
heptanal		114.18	? (read-across to be used) *900 µg/m³*
butanal		72.11	650 µg/m³ (de novo protocol) Unrounded value: 662.1 µg/m³ or 223.2 ppb

- Unrounded EU-LCI value butanal: 662.1 µg/m³ → to be used for read-across EU-LCI of heptanal.
- Cut-off rule in place: difference in change length between the two homologue compounds is larger than two CH_2 groups per aliphatic chain → cut-off to hexanal.
- Thus, EU-LCI value for heptanal is 662.1 µg/m³. After MW conversion at 23 °C and 1.013 atm (+ cut-off rule at 2C): EU-LCI heptanal = 662.1 µg/m3 x 1.39 = 920.3 µg/m³ → rounded to 900 µg/m³.
- The EU-LCI is above the odour detection threshold of ~ 2 µg/m³.

References

Nagata Y (2003) Measurement of odor threshold by triangle odor bag method. Odor Measurement Rev 118-127.