

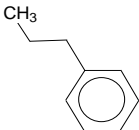
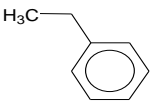
Compound	n-Propylbenzene (read-across from Ethylbenzene)		Factsheet
Parameter	Note	Comments	Value / descriptor
<b>EU-LCI Value and Status</b>			
EU-LCI value	1	Mass/volume [ $\mu\text{g}/\text{m}^3$ ]	950
EU-LCI status	2	Draft / Final	Final
EU-LCI year of issue	3	Year when the EU-LCI value has been issued	2013
<b>General Information</b>			
CLP-INDEX-Nr.	4	INDEX	601-024-00-X
EC-Nr.	5	EINECS – ELINCS - NLP	203-132-9
CAS-Nr.	6	Chemical Abstract Service number	103-65-1
Harmonised CLP classification	7	Human Health Risk related classification	Asp. Tox. 1 STOT SE 3
Molar mass	8	[g/mol]	120.19
<b>Key Data / Database</b>			
Key study, Author(s), Year	9	Critical study with lowest relevant effect level	
Read across compound	10	Where applicable	Ethylbenzene
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 Ethylbenzene
POD Value	17	[mg/m <sup>3</sup> ] or [ppm]	0.860 mg/m <sup>3</sup> and 0.197 ppm
<b>Assessment Factors (AF)</b>			
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	1.13 (=120.19/106.17)
Rounded value	30	$[\mu\text{g}/\text{m}^3]$	950
Additional Comments	31		

## Rationale Section

### Rationale for read-across

- Data poor compound: no adequate toxicological data for n-propylbenzene; *de novo* derivation of EU-LCI for n-propylbenzene is not possible.
- Read-across from EU-LCI value of ethylbenzene: within the chemical class 'saturated aromatic hydrocarbons', ethylbenzene is the closest homologue compound with an EU-LCI value: one additional  $\text{CH}_2$  group in the aliphatic side chain of n-propylbenzene.
- Toxicological critical endpoint for ethylbenzene: ototoxicity.
- The key assumption underlying the read-across of the EU-LCI value from ethylbenzene to propylbenzene is that both compounds have the same critical endpoint (ototoxicity) and this is caused by the common functional group (and not by the additional  $\text{CH}_2$  group).

Compound	Structure	MW [g/mol]	EU-LCI value
n-Propylbenzene		120.19	? (read-across to be used)  $950 \mu\text{g}/\text{m}^3$
Ethylbenzene		106.17	$850 \mu\text{g}/\text{m}^3$ (de novo protocol) Unrounded value: $860.6 \mu\text{g}/\text{m}^3$ or 197 ppb

- Unrounded EU-LCI value for ethylbenzene:  $860 \mu\text{g}/\text{m}^3 \rightarrow$  to be used for read-across EU-LCI of n-propylbenzene.  
No cut-off rule in place: difference in chain length between the two homologue compounds is smaller than two  $\text{CH}_2$  groups per aliphatic chain.
- Thus, EU-LCI value for ethylbenzene is  $860 \mu\text{g}/\text{m}^3$ . After MW conversion 23 °C and 1.013 atm: EU-LCI n-propylbenzene =  $860 \mu\text{g}/\text{m}^3 \times 1.13 = 971.8 \mu\text{g}/\text{m}^3 \rightarrow$  rounded to  $950 \mu\text{g}/\text{m}^3$ .