Compound	n-Butylbenzene (read-across from Ethylbenzene)		Factsheet
Parameter	**Note**	**Comments**	**Value / descriptor**
EU-LCI value and status			
EU-LCI value	1	Mass/volume [µg/m^3]	1100
EU-LCI status	2	Draft/final	Final
EU-LCI year of issue	3	Year when the EU-LCI value was issued	2014
General information			
CLP Index No	4	INDEX	(Not in Annex VI of CLP Regulation 1272/2008)
EC No	5	EINECS – ELINCS - NLP	203-209-7
CAS No	6	Chemical Abstract Service number	104-51-8
Harmonised CLP classification	7	Human health risk-related classification	Not harmonised
Molar mass and conversion factor	8	[g/mol] and [ppm – mg/m^3]	134.22 1 ppm = 5.52 mg/m^3
Key data / database			
Key study, author(s), year	9	Critical study with lowest relevant effect level	
Read-across compound	10	Where applicable	Ethylbenzene
Species	11	Rat etc. / human	
Route/type of study	12	Inhalation, oral feed, etc.	
Study length	13	Days, subchronic, chronic	
Exposure duration	14	Hours/day, days/week	
Critical endpoint	15	Effect(s), site of	
Point of departure (POD)	16	LOAEC*L, NOAEC*L, NOEC*L, benchmark dose, etc.	POD/TAF in EU-LCI factsheet for ethylbenzene
POD value	17	[mg/m^3] or [ppm] or [mg/kg$_{BW}$×d]	0.878 mg/m^3 or 0.2 ppm
Assessment factors (AF)	**18**		
Adjustment for exposure duration	19	Study exposure hours/day, days/week	-
Study Length	20	sa→ sc→ c *(R8-5)*	-
Route-to-route extrapolation factor	21		-
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)	878.3 µg/m³ 201 ppb
Molar adjustment factor	29	Used in read-across	1.264 (=134.22/106.17)
Rounded value	30	[µg/m³]	1100
Additional comments	31		
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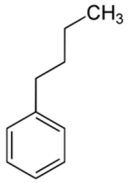
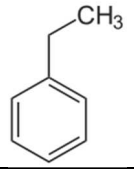
Rationale for read-across

- Data-poor compound: no adequate toxicological data for n-butylbenzene; *de novo* derivation of EU-LCI is not possible.
- Read-across candidate compounds for starting value: within the chemical class of 'saturated aromatic hydrocarbons', ethylbenzene is the closest homologue with an EU-LCI value.
- Toxicological critical endpoints for homologue compound:
  - ethylbenzene: ototoxicity.
- The key assumption underlying the read-across of the EU-LCI value from ethylbenzene to n-butylbenzene is that both compounds have the same critical endpoint and this endpoint is caused by the common functional group (and not by the additional CH_2 groups).

  The chemical structure and molecular weight of n-butylbenzene and ethylbenzene are listed in the table below:

Compounds	Structure	MW [g/mol]	EU-LCI value
n-Butylbenzene		134.22	? (read-across to be used)
Ethylbenzene		106.17	850 µg/m³ (*de novo* protocol) Unrounded value: 878.3 µg/m³ or 201 ppb

- No cut-off rule in place: the difference in change length between the two homologue compounds is smaller than two CH_2 groups per aliphatic chain.
- Thus, after EU-LCI n-butylbenzene = 878.3 µg/m³ x 1.264 = 1 110.17 µg/m³ → to be rounded to 1 100 µg/m³.