

Compound	2-Hexenal (read-across from 2-Butenal)		Factsheet
Parameter	Note	Comments	Value / descriptor
<b>EU-LCI value and status</b>			
EU-LCI value	1	Mass/volume [ $\mu\text{g}/\text{m}^3$ ]	7
EU-LCI status	2	Draft/final	Final
EU-LCI year of issue	3	Year when the EU-LCI value was issued	2015
<b>General information</b>			
CLP Index No	4	INDEX	-
EC No	5	EINECS — ELINCS — NLP	229-778-1
CAS No	6	Chemical Abstracts Service number	6728-26-3 (trans-2-hexenal) 16635-54-4 (cis-2-hexenal) 505-57-7 (undefined)
Harmonised CLP classification	7	Human health risk-related classification	Non harmonised substance
Molar mass and conversion factor	8	[g/mol] and [ppm — $\text{mg}/\text{m}^3$ ]	98.14 1 ppm = 4.03 $\text{mg}/\text{m}^3$
<b>Key data / database</b>			
Key study, author(s), year	9	Critical study with lowest relevant effect level	
Read-across compound	10	Where applicable	2-butenal
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 2-butenal
POD value	17	[ $\text{mg}/\text{m}^3$ ] or [ppm] or [ $\text{mg}/\text{kg}_{\text{BW}} \times \text{d}$ ]	0.002 ppm or 0.005 $\text{mg}/\text{m}^3$
<b>Assessment factors (AF)</b>			
Adjustment for exposure duration	19	Study exposure hours/day, days/week	-
Study length	20	sa $\rightarrow$ sc $\rightarrow$ c (R8-5)	-
Route-to-route extrapolation factor	21		-
Dose-response	22 a	Reliability of dose-response, LOAEL $\rightarrow$ 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)	-

<b>Result</b>			
Summary of assessment factors	27	Total Assessment Factor (TAF)	
POD/TAF	28	Calculated value ( $\mu\text{g}/\text{m}^3$ <u>and</u> ppb)	5.31 $\mu\text{g}/\text{m}^3$ and 1.85 ppb
Molar adjustment factor	29	Used in read-across	1.4 (= 98.14/70.08)
Rounded value	30	$[\mu\text{g}/\text{m}^3]$	7
<b>Additional comments</b>	31		
<b>Rationale section</b>	32		
<p><b>Rationale for read-across and assessment factors</b></p> <ul style="list-style-type: none"> <li>Given the lack of data to perform a de novo LCI derivation, the derivation of the LCI value for 2-hexenal is based on read-across from 2-butenal.</li> <li>Read-across candidate compounds for starting value: within the chemical class of 'unsaturated aldehydes' 2-butenal is the closest homologue. For this purpose, an EU-LCI value for 2-butenal was derived.</li> <li>Toxicological critical endpoints for homologue compound: <ul style="list-style-type: none"> <li>2-butenal: irritation</li> <li>The key assumption underlying the read-across of the EU-LCI value from 2-butenal to 2-hexenal is that both compounds have the same critical endpoint.</li> </ul> </li> <li>No cut-off rule in place: difference in chain length between the two homologue compounds is lower than two <math>\text{CH}_2</math> groups per aliphatic chain.</li> </ul> <p>Thus, the unrounded EU-LCI value for 2-hexenal is <math>5.31 \times 1.4 = 7.436 \mu\text{g}/\text{m}^3 \rightarrow</math> to be rounded to <math>7 \mu\text{g}/\text{m}^3</math>.</p>			