2-Heptylidene cyclopentan-1-one

CAS N°: 39189-74-7 **Empirical formula:** $C_{12}H_{20}O$

Synonyms: 2-Heptylidenecyclopentanone
2-Heptylidenecyclopentan-1-one
Cyclopentanone, 2-heptylidene-

Structure:

History:

Initial reviews:	New Standard	
Current revision date:	June 20, 2011	
Implementation date:	For new submissions*:	August 20, 2011
	For existing fragrance compounds*:	August 20, 2012
Next review date:	2016	

* This date applies to the supply of fragrance compounds (formulas) only, not to the finished products in the marketplace.

RECOMMENDATION: RESTRICTED

RESTRICTIONS:

Limits in the finished product:			
Category 1 See Note box (1)	0.03%	Category 7	0.08%
Category 2	0.04%	Category 8	1.01%
Category 3	0.15%	Category 9	5.00%
Category 4	0.45%	Category 10	2.50%
Category 5	0.24%	Category 11	See Note box (2)
Category 6 See Note box (1)	0.72%		

Note box:
(1) See the IFRA Code of Practice (Appendix 8, Introduction to the IFRA Standards) regarding the Note on Oral Care Products and other products with the potential of ingestion.
(2) Category 11 includes all non-skin contact or incidental skin contact products. Due to the negligible skin contact from these types of products there is no justification for a restriction of the concentration of this fragrance ingredient in the finished product.

Fragrance material specifications: N/A

Indicative contribution from other sources: None known at the time of the publication of the Standard

Critical effect: Sensitization

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RIFM Summaries:

LLNA weighted mean EC3 values ($\mu g/cm^2$) [no. studies]	Potency Classification Based on Animal Data[1]	Human Data[2]			WoE NESIL[3] ($\mu g/cm^2$)
		NOEL – HRIPT (induction) ($\mu g/cm^2$)	NOEL – HMT (induction) ($\mu g/cm^2$)	LOEL (induction) ($\mu g/cm^2$)	
4100 [1]	Weak	NA	NA	NA	1000

All data in this Table are available from RIFM and are listed in the RIFM Database.
NOEL = No observed effect level; HRIPT = Human Repeat Insult Patch Test; HMT = Human Maximization Test; LOEL = lowest observed effect level; NA = Not Available.

[1]Based on animal data using classification defined in ECETOC, Technical Report No. 87, 2003.
[2]Data derived from HRIPT or HMT.
[3]WoE NESIL limited to two significant figures.

REXPAN Rationale / Conclusion:

The RIFM Expert Panel reviewed the critical effect data for 2-Heptylidene cyclopentan-1-one and, based on the weight of evidence, established the No Expected Sensitization Induction Level (NESIL) as 1000 $\mu g/cm^2$, which is a default value based on the LLNA data. They recommend the limits for the 11 different product categories, which are the acceptable use levels of 2-Heptylidene cyclopentan-1-one in the various product categories. These were derived from the application of the exposure-based quantitative risk assessment approach for fragrance ingredients, which is detailed in the publication by Api *et al*., 2008.

References:

Api AM, Basketter DA, Cadby PA, Cano M-F, Ellis G, Gerberick G, et al. Dermal Sensitization Quantitative Risk Assessment (QRA) For Fragrance Ingredients. *Regulatory Toxicology and Pharmacology* 2008;52(1): 3-23.