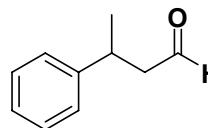


3-Phenylbutanal

CAS N°: 16251-77-7**Empirical formula:** C₁₀H₁₂O

Synonyms: Benzenepropanal, β-methyl-
3-Phenylbutanal
3-Phenylbutyraldehyde
3-Phenyl-3-methylpropanal
Trifernal (commercial name)

Structure:**History:**

Initial reviews: New Standard

Current revision date: June 11, 2010

Implementation date: For new submissions*: August 11, 2010For existing fragrance compounds*: August 11, 2011**Next review date:** 2015

* 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)	0.17%	Category 7	0.45%
Category 2		0.22%	Category 8	2.0%
Category 3		0.89%	Category 9	5.0%
Category 4		2.7%	Category 10	2.5%
Category 5		1.4%	Category 11	See Note box (2)
Category 6	See Note box (1)	4.3%		
<u>Note box:</u> (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.				
<u>Fragrance material specifications:</u> N/A				

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

Critical effect: Sensitization

3-Phenylbutanal

RIFM Summaries:

LLNA weighted mean EC3 values (µg/cm ²) [no. studies]	Potency Classification Based on Animal Data ¹	Human Data ²			WoE NESIL ³ (µg/cm ²)
		NOEL – HRIPT (induction) (µg/cm ²)	NOEL – HMT (induction) (µg/cm ²)	LOEL (induction) (µg/cm ²)	
N/A	N/A	5906	N/A	12,500	5900

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.

¹Based on animal data using classification defined in ECETOC, Technical Report No. 87, 2003.

²Data derived from HRIPT or HMT.

³WoE NESIL limited to two significant figures.

REXPAN Rationale / Conclusion:

The RIFM Expert Panel reviewed the critical effect data for 3-phenylbutanal and, based on the weight of evidence, established the No Expected Sensitization Induction Level (NESIL) as 5900 µg/cm². They recommend the limits for the 11 different product categories, which are the acceptable use levels of 3-phenylbutanal 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.

RIFM (Research Institute for Fragrance Materials, Inc.), 2009. Human repeated insult patch test. RIFM report number 57513, July 16. (RIFM, Woodcliff Lake, NJ, USA).

RIFM (Research Institute for Fragrance Materials, Inc.), 1983. Human repeated insult patch test. Unpublished study from Firmenich, Inc., August 24. Report number 40514. (RIFM, Woodcliff Lake, NJ, USA).