Methyl ionone, mixed isomers

CAS N°: **Empirical formula:** $C_{14}H_{22}O$

Synonyms: 1335-46-2 Methyl ionone, mixture of isomers
127-42-4 Methyl-alpha-ionone
alpha-Cetone
alpha-Cyclocitrylidenebutanone
alpha-Cyclocitrylidenemethyl ethyl ketone
Methyl-a-ionone
alpha-Methylionone
1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, [R-(E)]-
(R-(E))-1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one
127-43-5 Methyl-beta-ionone
Methyl-ß-ionone
beta-Methylionone
beta-Cetone
beta-Cyclocitrylidenebutanone
beta-Iraldeine
1-Penten-3-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-
5-(2,6,6-Trimethyl-1-cyclohexen-1-yl)-4-penten-3-one
1-(2,6,6-Trimethyl-1-cyclohexen-1-yl)pent -1-en-3-one
127-51-5 alpha-iso methylionone
3-Buten-2-one, 3-methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-
3-Methyl-4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-3-buten-2-one
alpha-Isomethyl ionone
gamma-Methylionone
Iraldeine gamma
Isoraldeine 95
7779-30-8 1-(2,6,6-Trimethyl-2-cyclohexen-1-yl)pent-1-en-3-one
1-Penten-3-one, 1-(2,6,6-trimethyl-2-cyclohexen-1-yl)-

History:			
	Initial reviews:	2007 (42nd Amendment)	
	Current revision date:	2008	
	Implementation date:	For new submissions*:	August 16, 2008
		For existing fragrance compounds*:	August 16, 2010
	Next review date:	2013	

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

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Standard: RESTRICTED

RESTRICTIONS:

Limits in the finished product:
For a description of the categories, refer to the QRA Informational Booklet.

Category 1: See Note Box (1)	2 %	Category 7:	5.3 %
Category 2:	2.6 %	Category 8:	2 %
Category 3:	10.6 %	Category 9:	5 %
Category 4:	31.7 %	Category 10:	2.5 %
Category 5:	16.7 %	Category 11: See Note Box (2)	
Category 6: See Note Box (1)	50.7 %		

Note box:
For this material, for pragmatic reasons, restrictive levels allowed by the QRA for certain categories but actually being higher than those already in place before applying the QRA, will temporarily not be implemented until the end of a 5 year monitoring phase. At the end of the 5 years the position will be reevaluated again.

(1) IFRA would recommend that any material used to impart perfume or flavour in products intended for human ingestion should consist of ingredients that are in compliance with appropriate regulations for foods and food flavourings in the countries of planned distribution and, where these are lacking, with the recommendations laid down in the Code of Practice of IOFI (International Organisation of the Flavor Industry). Further information about IOFI can be found on its website (http://www.iofiorg.org/).

(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.

The above limits apply to methyl ionone isomers used individually or in combination.

Fragrance material specification: N/A

Contribution from other sources: None to consider (See also the note on contributions from other sources in the Introduction to the IFRA Standards)

Critical effect: Sensitization

Methyl ionone, mixed isomers

RIFM Summaries:

EC_3 value from one **LLNA** (not the mean) ($\mu g/cm^2$) [No. Studies]	**Potency Classification** Based on Animal Data[1]	**Human Data**			**WoE NESIL[3]** ($\mu g/cm^2$)
		NOEL – HRIPT (induction) ($\mu g/cm^2$)	**NOEL – HMT** (induction) ($\mu g/cm^2$)	**LOEL[2]** (induction) ($\mu g/cm^2$)	
5450	Weak	70866[4]	NA	NA	70000

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 three significant figures

[4] MT-NOEL = Maximum Tested No Effect Level. No sensitization was observed in human predictive studies. Doses reported reflect the highest concentration tested, not necessarily the highest achievable NOEL

REXPAN Rationale / Conclusion:

The RIFM Expert Panel reviewed the critical effect data for Methyl ionone, mixed isomers and, based on the weight of evidence, established the No Expected Sensitization Induction Level (NESIL) as 70000 µg/cm². They recommend the limits for the 11 different product categories, which are the acceptable use levels of Methyl ionone, mixed isomers 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 QRA Expert Group Technical Dossier of June 22, 2006.

References:

RIFM (Research Institute for Fragrance Materials, Inc.), 2004a. Repeated insult patch test with alpha-iso-methylionone. RIFM report number 47278, March 10. (RIFM, Woodcliff Lake, NJ, USA).

RIFM (Research Institute for Fragrance Materials, Inc.), 2004b. Repeated insult patch test with alpha-iso-methylionone. RIFM report number 47279, March 10. (RIFM, Woodcliff Lake, NJ, USA).

RIFM (Research Institute for Fragrance Materials, Inc.), 2005. alpha-iso-Methylionone diluted with vehicle 1:3 EtOH:DEP: Local Lymph Node Assay. RIFM report number 48749, January 26. (RIFM, Woodcliff Lake, NJ, USA).