Methyl heptine carbonate

CAS N°: 111-12-6 **Empirical formula:** $C_9H_{14}O_2$

Synonyms: Methyl heptyne carbonate
Methyl 2-octynoate
MHC
2-Octynoic acid, methyl ester
Folione

History:

Initial reviews:	October 1976, April 2000, April 2005 (39th Amendment, new format only)	
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.

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)	0.003 %	Category 7:	0.008 %
Category 2:	0.004 %	Category 8:	0.01 %
Category 3:	0.01 %	Category 9:	0.01 %
Category 4:	0.01 %	Category 10:	0.01 %
Category 5:	0.01 %	Category 11: Not Restricted (2)	
Category 6: See Note box (1)	0.08 %		

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) 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.

When used in the same fragrance compound within a specific QRA category, the sum total of methyl heptine carbonate (MHC) and methyl octine carbonate (MOC) contributions must not exceed the maximum permitted level for MHC. At the same time, the contribution

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from methyl octine carbonate should always respect the maximum levels permitted in the respective categories as listed in the Standard for MOC.
If the same compound is intended for more than one IFRA QRA category, then the most restrictive limitations (based on foreseen use concentrations and maximum permitted level) will apply.

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

RIFM Summaries:

EC3 value from one **LLNA** (not the mean) ($\mu g/cm^2$)	**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) ($\mu g/cm^2$)	
< 125	Strong	118 [4]	NA	194	110

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 heptine carbonate and, based on the weight of evidence, established the No Expected Sensitization Induction Level (NESIL) as 110 mg/cm2. They recommend the limits for the 11 different product categories, which are the acceptable use levels of methyl heptine carbonate 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.), 1964. Human repeated patch test on methyl-2-nonynoate and isoeugenol. Unpublished report from IFF, Inc., 30 April. Report number 1808. (RIFM, Woodcliff Lake, NJ, USA).

RIFM (Research Institute for Fragrance Materials, Inc.), 1989. Human repeated insult patch test of methyl 2-octynoate. RIFM report number 12368, November 16. (RIFM, Woodcliff Lake, NJ, USA).

RIFM (Research Institute for Fragrance Materials, Inc.), 1990. Repeated insult patch test of methyl 2-octynoate in human subjects. RIFM report number 12452, April 27. (RIFM, Woodcliff Lake, NJ, USA).

RIFM (Research Institute for Fragrance Materials, Inc.), 2005. Methyl 2-octynoate diluted

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with vehicle 1:3 EtOH:DEP: Local Lymph Node Assay. RIFM report number 48753, January 28. (RIFM, Woodcliff Lake, NJ, USA).

RIFM (Research Institute for Fragrance Materials, Inc.), 2006. Methyl 2-octynoate: Local Lymph Node Assay. RIFM report number 51627, April 6. (RIFM, Woodcliff Lake, NJ, USA).