VETIVERYL ACETATE

CAS N°: 117-98-6
62563-80-8
68917-34-0
73246-97-6
84082-84-8

Empirical formula: $C_{17}H_{26}O_2$

Synonyms: 6-Azulenol, 1,2,3,3a,4,5,6,8a-octahydro-4,8-dimethyl-2-(methylethylidene)-, acetate
6-Azulenol, 1,2,3,3a,4,5,6,8a-octahydro-4,8-dimethyl-2-(1-methylethylidene)-, acetate
2-Isopropylidene-4,8-dimethyl-1,2,3,3a,4,5,6,8a-octahydroazulen-6-yl acetate
Vetivert acetate, Vetivert acetate (Haiti), Vetyvenyl acetate
Vetiverol, acetate

History:

Initial reviews:	New Standard	
Current revision date:	2009	
Implementation date:	for new submissions*:	August 7, 2009
	for existing fragrance compounds*:	August 7, 2011
Next review date:	2014	

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

STANDARD: RESTRICTED / SPECIFICATION

RESTRICTIONS:

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

Category 1 - See Note box (1)	0.07 %	Category 7	0.17 %
Category 2	0.08 %	Category 8	2.00 %
Category 3	0.35 %	Category 9	5.00 %
Category 4	1.04 %	Category 10	2.50 %
Category 5	0.55 %	Category 11	See Note box (2)
Category 6 - See Note box (1)	1.67 %		

Note box:
(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 - www.iofiorg.org)

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(2) Category 11 includes all non-skin contact or incidental skin contact products. Due to negligible skin contact the concentration of a fragrance ingredient should not exceed the usual concentration of the fragrance compound in the finished product.

Fragrance material specification:

Acetylated vetiver oil (Vetiveryl acetate) should only be used as a fragrance ingredient if produced by methods that lead to a reduction in allergenic materials, like the ones outlined below (acetylation methods using acetic anhydride):

- without catalyst, at a temperature not exceeding 120℃.
- with ortho phosphoric acid at room temperature.
- with sodium acetate in toluene at reflux temperature.

The first two products can be used in their crude form after the usual procedures, but may be further purified. In the last case, distillation is necessary.
Another method accepted is an enzymatic acetylation process.
This recommendation is based on test results of RIFM with samples prepared according to different acetylation methods (private communication to IFRA).

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

Critical effect: Sensitization

RIFM Summaries:

LLNA weighted mean EC3 values ($\mu g/cm^2$) [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) ($\mu g/cm^2$)	
2910 [4]	Weak	2362	NA	NA	2300

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

REXPAN Rationale / Conclusion:

The RIFM Expert Panel reviewed the critical effect data for Vetiveryl acetate and, based on the weight of evidence, established the No Expected Sensitization Induction Level (NESIL) as 2300 $\mu g/cm^2$. They recommend the limits for the 11 different product categories, which are the acceptable use levels of Vetiveryl acetate 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.

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References:

Jones, L., Foxenberg, R., Lalko, J., Letizia, C., Api, A, 2008. Sensitization potential of vetiveryl acetate evaluated using the Local Lymph Node Assay. The Toxicologist, 102, 298.

RIFM (Research Institute for Fragrance Materials, Inc.), 2008. Local Lymph Node Assay. RIFM report number 55336, July 29. (RIFM, Woodcliff Lake, NJ, USA).