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Review

Fragrance material review on tricyclodecenyl acetate

S.P. Bhatia *, L. Jones, C.S. Letizia, A.M. Api

Research Institute for Fragrance Materials, Inc., 50 Tice Boulevard, Woodcliff Lake, NJ 07677, USA

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ABSTRACT

A toxicologic and dermatologic review of tricyclodecenyl acetate when used as a fragrance ingredient is presented.

Contents

Introduction

In 2007, a complete literature search was conducted on tricyclodecenyl acetate. On-line databases that were surveyed included Chemical Abstract Services and the National Library of Medicine. In addition, fragrance companies were asked to submit pertinent test data. All relevant references are included in this document. Any papers in which the vehicles and/or the doses are not given have not been included in this review. The number of animals, sex and strain are always provided unless they are not given in the original report or paper.

This individual Fragrance Material Review is not intended as a stand-alone document. Please refer to the Toxicologic and

* Corresponding author. Tel.: +1 201 689 8089; fax: +1 201 689 8070.
E-mail address: sbhatia@rifm.org (S.P. Bhatia).

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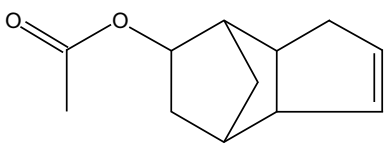

Fig. 1. Tricyclodecenyl acetate.

Dermatologic Assessment of Cyclic Acetates (Belsito et al., 2008) for an overall assessment of this material.

1. Identification (Fig. 1)

1.1 Synonyms: dihydronorbicyclopentadienyl acetate; greenylacetate; herbaflorat; 3a,4,5,6,7,7a-hexahydro-4,7-methanoinden-6-ylacetate; jasmacyclene; 4,7-methano-1*H*-inden-6-ol-3a,4,5,6,7,7a-hexahydro acetate; tricyclodecen-4-yl 8-acetate; verdyl acetate.
1.2 CAS Registry Number: 5413-60-5.
1.3 EINECS number: 226-501-6.
1.4 Formula: $C_{12}H_{16}O_2$.
1.5 Molecular weight: 192.26.

2. Physical properties

2.1 Physical form: a colorless viscous liquid.
2.2 Acid value: free.
2.3 Purity: 96.6%.
2.4 Flash point: >200 °F; CC.
2.5 Henry's law: 0.000169 atm m^3/mol at 25 °C.
2.6 Log K_{ow}: 3.19 (calculated); 3.8 (measured at 25 °C).
2.7 Refractive index: 1.4950.
2.8 Specific gravity: 1.072.
2.9 Specific gravity: 1.0735.
2.10 Vapor pressure (calculated): 0.0758 mm Hg at 25 °C.
2.11 Water solubility (calculated) 177.4 mg at 25 °C.

3. Usage

Tricyclodecenyl acetate is a fragrance ingredient used in many fragrance compounds. It may be found in fragrances used in decorative cosmetics, fine fragrances, shampoos, toilet soaps and other toiletries as well as in non-cosmetic products such as household cleaners and detergents. Its use worldwide is in the region of 100–1000 metric tonnes per annum.

The maximum skin level that results from the use of tricyclodecenyl acetate in formulae that go into fine fragrances has been reported to be 1.18% assuming use of the fragrance oil at levels up to 20% in the final product. The 97.5 percentile use level in formulae for use in cosmetics in general has been reported to be 4.41% (IFRA, 2007), which would result in a conservative calculated maximum daily exposure on the skin of 0.1124 mg/kg for high end users of these products (see Table 1).

4. Toxicology data

4.1. Acute toxicity

See Table 2.

4.1.1. Oral studies

4.1.1.1. The acute oral LD_{50} in 10 rats was determined to exceed 5 g/kg. Ten rats were orally dose with tricyclodecenyl acetate at 5 g/kg. Observations were made for 14 days. Clinical signs included flaccid tone, lethargy, ataxia, and ptosis. Death occurred in 2/10 rats on days 11 and 12. Necropsy observations in rats that died included yellow intestines, dark lungs, blotchy liver, and small spleen. Necropsy observations in rats sacrificed after 14 days included dried blood around nose (3 rats) and small spleen (1 rat) (RIFM, 1977a).

4.1.1.2. The acute oral LD_{50} of tricyclodecenyl acetate in rats was reported to be >5 g/kg. Mortality was 1 of 10 rats at 5 g/kg. Death occurred on day 1. Slight lethargy was the only clinical sign observed. No additional details were reported (RIFM, 1974a).

4.1.1.3. The acute oral LD_{50} of tricyclodecenyl acetate in healthy female Holtzman strain rats (10/dose) was reported to be 4 ml/kg (~4.3 g/kg). Animals were dosed intragastrically with test material at 2, 4, 5, 6.5, and 8.0 ml/kg (~1.07, 2.14, 4.3, 5.4, 7, and 8.6 g/kg). Death occurred in 1/10, 6/10, 7/10, 8/10, and 10/10 animals at 2, 4, 5, 6.5, and 8.0 ml/kg, respectively. Death occurred with 24–72 h after administration (RIFM, 1958).

4.1.1.4. The acute oral LD_{50} of tricyclodecenyl acetate in mice was reported to be approximately 5 ml/kg (~5.4 g/kg). The test material was orally administered to mice (2–6 per group) at 2, 5 and 10 ml/kg (~2.14, 5.4, and 10.7 g/kg). Observations were made for 7 days. Clinical signs included convulsions, cyanosis, labored breathing, somnolence, and semi-comatose state. Death occurred in 2/2 mice at 5 ml/kg and 3/6 at 10 ml/kg. Necropsy findings in mice that died included dark brown fluid in intestines, irritation in duodenum and ileum, pale grey fluid in the caeca, and pale

Table 1
Calculation of the total human skin exposure from the use of multiple cosmetic products containing tricyclodecenyl acetate

Type of cosmetic product	Grams applied	Applications per day	Retention factor	Mixture/product	Ingredient/mixture[a]	Ingredient (mg/kg/day)[b]
Anti-perspirant	0.50	1.00	1.00	0.01	4.41	0.0037
Bath products	17.00	0.29	0.001	0.02	4.41	0.0001
Body lotion	8.00	0.71	1.00	0.004	4.41	0.0167
Eau de toilette	0.75	1.00	1.00	0.08	4.41	0.0441
Face cream	0.80	2.00	1.00	0.003	4.41	0.0035
Fragrance cream	5.00	0.29	1.00	0.04	4.41	0.0426
Hair spray	5.00	2.00	0.01	0.005	4.41	0.0004
Shampoo	8.00	1.00	0.01	0.005	4.41	0.0003
Shower gel	5.00	1.07	0.01	0.012	4.41	0.0005
Toilet soap	0.8	6.00	0.01	0.015	4.41	0.0005
Total						0.1124

[a] Upper 97.5 percentile levels of the fragrance ingredient in the fragrance mixture used in these products.
[b] Based on a 60 kg adult.