Food and Chemical Toxicology 46 (2008) S102–S105

Contents lists available at ScienceDirect

Food and Chemical Toxicology

journal homepage: www.elsevier.com/locate/foodchemtox

Review

Fragrance material review on 1,7,7-trimethylbicyclo[4.4.0]dec-3-yl acetate

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

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

ARTICLE INFO

Keywords:
Fragrance material
Review
1,7,7-trimethylbicyclo[4.4.0]dec-3-yl acetate

ABSTRACT

A toxicologic and dermatologic review of 1,7,7-trimethylbicyclo[4.4.0]dec-3-yl acetate when used as a fragrance ingredient is presented.

Contents

Introduction

In 2007, a complete literature search was conducted on 1,7,7-trimethylbicyclo[4.4.0]dec-3-yl acetate. On-line databases that were surveyed included Chemical Abstract Services and the National Library of Medicine. In addition, fragrance companies

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

0278-6915/$ - see front matter © 2008 Elsevier Ltd. All rights reserved.
doi:10.1016/j.fct.2008.09.020

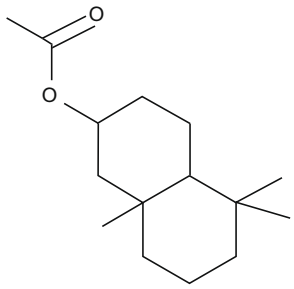

Fig. 1. 1,7,7-Trimethylbicyclo[4.4.0]dec-3-yl acetate.

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

1. Identification (Fig. 1)

1.1 Synonyms: decahydro-5,5,8a-trimethyl-2-naphthyl acetate; 2-naphthalenol, decahydro-5,5,8a-trimethyl-, acetate; 2-naphthol, decahydro-5,5,8a-trimethyl-, acetate; polywood; 1,7,7-trimethylbicyclo[4.4.0]decan-3-yl acetate.
1.2 CAS Registry Number: 24238-95-7.
1.3 EINECS Number: 246-105-7.
1.4 Formula: $C_{15}H_{26}O_2$.
1.5 Molecular weight: 238.37.

2. Physical properties

2.1 Flash point: 100 °C.
2.2 Log K_{ow} (calculated): 4.99.
2.3 Vapor pressure (calculated): 0.00187 mm Hg at 25 °C.
2.4 Water solubility (calculated): 1.507 mg/l at 25 °C.
2.5 Refractive Index: 1.4760 at 20 °C.
2.6 Henry's Law (calculated): 0.00102 atm m^3/mol at 25 °C.
2.7 Density: 0.9758 d20/20.

3. Usage

1,7,7-Trimethylbicyclo[4.4.0]dec-3-yl 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 0.1–1 metric tonnes per annum.

The maximum skin level that results from the use of 1,7,7-trimethylbicyclo[4.4.0]dec-3-yl acetate in formulae that go into fine fragrances has not been reported. A default value of 0.02% is used, 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 not been reported. As such the default value of 0.02% is used to calculate the maximum daily exposure on the skin of 0.0005 mg/kg for high end users of these products (see Table 1).

Table 2
Summary of acute toxicity data

Route	Species	No. animals/dose group	LD_{50} (g/kg)	References
Oral	Rat	10	>5	RIFM (1979a)
Dermal	Rabbit	6	>2	RIFM (1979b)

4. Toxicology data

4.1. Acute toxicity

See Table 2.

4.1.1. Oral studies

4.1.1.1. Ten male and female (5/sex/dose) Sherman-Wistar albino rats received single oral administration of 5 g/kg test material. Animals were observed for signs of toxicity and morality for 14 days. One animal (1/10) died within first 6 h. Within 2–3 h animals appeared slightly lethargic and ataxic. All surviving animals appeared normal after 48 h. The acute oral LD_{50} in rats was reported to exceed 5.0 g/kg (RIFM, 1979a).

4.1.2. Dermal studies

4.1.2.1. The acute dermal LD_{50} was reported to be greater than 2 g/kg based on no death at that dose. Six rabbits (3/sex) received a single dermal application of neat test material for 24 h under occlusion. Animals were observed for 14 days. No clinical signs or deaths were observed (RIFM, 1979b).

4.2. Skin irritation

4.2.1. Human studies

4.2.1.1. Irritation was evaluated during the induction phase of human repeated insult patch test conducted on 50 volunteers (nine male and 41 female). A 0.2 g of 20% test material in petrolatum was applied to the upper arm of each subject and then covered with a semi-occlusive patch for 24 h. A total of nine 24-h applications were made over a three week period, based on

Table 1
Calculation of the total human skin exposure from the use of multiple cosmetic products containing 1,7,7-trimethylbicyclo[4.4.0]dec-3-yl acetate

Type of cosmetic product	Grams applied	Applications per day	Retention factor	Mixture/product	Ingredient/mixture[a]	Ingredient (mg/kg/day)[b]
Body lotion	8.00	0.71	1.000	0.004	0.02	0.0001
Face cream	0.80	2.00	1.000	0.003	0.02	0.0000
Eau de toilette	0.75	1.00	1.000	0.080	0.02	0.0002
Fragrance cream	5.00	0.29	1.000	0.040	0.02	0.0002
Antiperspirant	0.50	1.00	1.000	0.010	0.02	0.0000
Shampoo	8.00	1.00	0.010	0.005	0.02	0.0000
Bath products	17.00	0.29	0.001	0.020	0.02	0.0000
Shower gel	5.00	1.07	0.010	0.012	0.02	0.0000
Toilet soap	0.80	6.00	0.010	0.015	0.02	0.0000
Hair spray	5.00	2.00	0.010	0.005	0.02	0.0000
Total						0.0005

[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.