



Review

Fragrance material review on isotridecan-1-ol (isomeric mixture)

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ABSTRACT

A toxicologic and dermatologic review of isotridecan-1-ol (isomeric mixture) when used as a fragrance ingredient is presented. Isotridecan-1-ol (isomeric mixture) is a member of the fragrance structural group branched chain saturated alcohols. The common characteristic structural elements of the alcohols with saturated branched chain are one hydroxyl group per molecule, and a C₄–C₁₂ carbon chain with one or several methyl side chains. This review contains a detailed summary of all available toxicology and dermatology papers that are related to this individual fragrance ingredient and is not intended as a stand-alone document. A safety assessment of the entire branched chain saturated alcohol group will be published simultaneously with this document; please refer to [Belsito et al. \(2010\)](#) for an overall assessment of the safe use of this material and all other branched chain saturated alcohols in fragrances.

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Introduction

This document provides a summary of the toxicologic review, including all human health endpoints, of isotridecan-1-ol (isomeric

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mixture) when used as a fragrance ingredient. Isotridecan-1-ol (see Fig. 1; CAS Number 27458-92-0) is a fragrance ingredient used in cosmetics, fine fragrances, shampoos, toilet soaps and other toiletries as well as in non-cosmetic products such as household cleaners and detergents. This material has been reported to occur in nature within beef (VCF, 2009).

In 2006, a complete literature search was conducted on Isotridecan-1-ol. On-line toxicological databases were searched including those from the Chemical Abstract Services, [e.g., ToxCenter (which in itself contains 18 databases including Chemical Abstracts)], and the National Library of Medicine [e.g., Medline, Toxnet (which contains 14 databases)] as well as 26 additional sources (e.g., BIOSIS, Embase, RTECS, OSHA, ESI). In addition, fragrance companies were asked to submit all test data.

The safety data on this material has never been reviewed before by RIFM (Research Institute for Fragrance Materials, Inc.). All relevant references are included in this document. More details have been provided for unpublished data. The number of animals, sex and strain are always provided unless they are not given in the original report or paper. Any papers in which the vehicles and/or the doses are not given have not been included in this review. In addition, diagnostic patch test data with fewer than 100 consecutive patients have been omitted.

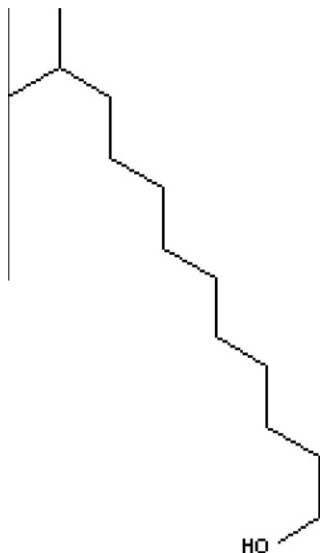


Fig. 1. Isotridecan-1-ol (isomeric mixture).

1. Identification

- 1.1 Synonyms: Isotridecanol; 11-methyldodecan-1-ol
- 1.2 CAS registry number: 27458-92-0
- 1.3 EINECS number: 248-469-2
- 1.4 Formula: $C_{13}H_{28}O$
- 1.5 Molecular weight: 200.66

2. Physical properties

- 2.1 Physical form: no information available
- 2.2 Boiling point (calculated; EPA, 2010): 279.35 °C
- 2.3 Flash point: no information available
- 2.4 Henry's law (calculated; EPA, 2010): 0.000128 atm m³/mol 25 °C
- 2.5 Log K_{ow} (calculated; EPA, 2010): 5.19
- 2.6 Refractive index: no information available
- 2.7 Specific gravity: no information available
- 2.8 Vapor pressure (calculated; EPA, 2010): 0.000462 mm Hg; 0.0615 Pa (25 °C)
- 2.9 Water solubility (calculated; EPA, 2010): 5.237 mg/l at 25°
- 2.10 UV spectra available at RIFM. Does not absorb UV light.

3. Usage

Isotridecan-1-ol (isomeric mixture) 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 10–100 metric tons per annum (IFRA, 2004). The reported volume of use is for isotridecan-1-ol as used in fragrance compounds (mixtures) in all finished consumer product categories. The volume of use is surveyed by IFRA approximately every four years through a comprehensive survey of IFRA and RIFM member companies. As such the volume of use data from this survey provides volume of use of fragrance ingredients for the majority of the fragrance industry.

The dermal systemic exposure in cosmetic products (see Table 1) is calculated based on the concentrations of the same fragrance ingredient in ten types of the most frequently used personal care and cosmetic products (anti-perspirant, bath products, body lotion, eau de toilette, face cream, fragrance cream, hair spray, shampoo, shower gel, and toilet soap). The concentration of the fragrance ingredient in fine fragrances is obtained from examination of several thousand commercial formulations. The upper 97.5 percentile concentration is calculated from the data obtained. This upper 97.5 percentile concentration is then used for all 10

Table 1

Calculation of the total human skin exposure from the use of multiple cosmetic products containing isotridecan-1-ol (isomeric mixture).

Product type	Grams applied	Applications per day	Retention factor	Mixture/product (%)	Ingredient/mixture ^a	Ingredient (mg/kg/day) ^b
Anti-perspirant	0.5	1	1	0.01	1.4	0.0012
Bath products	17	0.29	0.001	0.02	1.4	0.00002
Body lotion	8	0.71	1	0.004	1.4	0.0053
Eau de toilette	0.75	1	1	0.08	1.4	0.0140
Face cream	0.8	2	1	0.003	1.4	0.0011
Fragrance cream	5	0.29	1	0.04	1.4	0.0135
Hair spray	5	2	0.01	0.005	1.4	0.0001
Shampoo	8	1	0.01	0.005	1.4	0.0001
Shower gel	5	1.07	0.01	0.012	1.4	0.0001
Toilet soap	0.8	6	0.01	0.015	1.4	0.0002
Total						0.0357

^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.

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