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Review

Fragrance material review on 1-(3,3-dimethylbicyclo[2.2.1]hept-2-yl) ethane-1-one

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ABSTRACT

A toxicologic and dermatologic review of 1-(3,3-dimethylbicyclo[2.2.1]hept-2-yl)ethane-1-one when used as a fragrance ingredient is presented. 1-(3,3-Dimethylbicyclo[2.2.1]hept-2-yl)ethane-1-one is a member of the fragrance structural group Alkyl Cyclic Ketones. These fragrances can be described as being composed of an alkyl, R_1, and various substituted and bicyclic saturated or unsaturated cyclic hydrocarbons, R_2, in which one of the rings may include up to 12 carbons. Alternatively, R_2 may be a carbon bridge of C2–C4 carbon chain length between the ketone and cyclic hydrocarbon. 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. Available data for 1-(3,3-dimethylbicyclo[2.2.1]hept-2-yl)ethane-1-one were evaluated then summarized and includes physical properties, skin irritation, mucous membrane (eye) irritation, and skin sensitization data. A safety assessment of the entire Alkyl Cyclic Ketones will be published simultaneously with this document; please refer to Belsito et al. (Belsito, D., Bickers, D., Bruze, M., Calow, P., Dagli, M., Fryer, A.D., Greim, H., Miyachi, Y., Saurat, J.H., Sipes, I.G., 2013. A Toxicologic and Dermatologic Assessment of Alkyl Cyclic Ketones When Used as Fragrance Ingredients (submitted for publication) for an overall assessment of the safe use of this material and all Alkyl Cyclic Ketones in fragrances.

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Contents

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1. Introduction

This document provides a comprehensive summary of the human health toxicological data currently available pertaining to the safety evaluation of 1-(3,3-dimethylbicyclo[2.2.1]hept-2-yl)ethane-1-one (See Fig. 1) when used as a fragrance ingredient. All safety data on 1-(3,3-dimethylbicyclo[2.2.1]hept-2-yl)ethane-1-one were compiled with due diligence including published and unpublished data. In 2013, a complete literature search was conducted on 1-(3,3-dimethylbicyclo[2.2.1]hept-2-yl)ethane-1-one. 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, ESIS). In addition, all RIFM sponsored studies and studies from fragrance companies are included in this summary.

Data from all relevant references are summarized in this FMR. Commonly used terms and their abbreviations are listed in Appendix A. 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. Papers in which the vehicles and/or the doses are not given were included and noted in this summary because either they demonstrated an adverse effect or there were limited to no data on this fragrance ingredient.

2. Identification

2.1.

Synonyms: 1-(3,3-Dimethylbicyclo[2.2.1]hept-2-yl)ethanone; Ethanone, 1-(3,3-dimethylbicyclo[2.2.1]hept-2-yl)-; Camek DH

2.2.

CAS Registry Number: 42370-07-0

2.3.

EINECS Number: 255-779-1

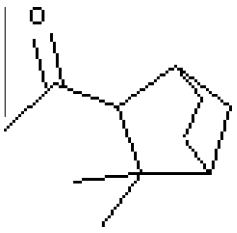

Fig. 1. 1-(3,3-Dimethylbicyclo[2.2.1]hept-2-yl)ethane-1-one.

2.4.

Formula: $C_{11}H_{18}O$

2.5.

Molecular Weight: 166.64

3. Physical properties[1]

3.1.

Boiling Point: 211 °C

3.2.

Henry's Law (calculated): 0.0000929 atm m^3/mol @ 25 °C

3.3.

Log K_{ow} (calculated): 2.80

3.4.

Vapor pressure (calculated): 0.303 mm Hg @ 25 °C

3.5.

Water Solubility (calculated): 262.5 mg/l @ 25 °C

3.6.

UV spectra not available at RIFM

4. Usage

1-(3,3-Dimethylbicyclo[2.2.1]hept-2-yl)ethane-1-one is a fragrance ingredient used in many 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. The worldwide volume of use for 1-(3,3-dimethylbicyclo[2.2.1]hept-2-yl)ethane-1-one is in the region of 0.1–1 metric tons per year (IFRA, 2008). This reported volume is for its use as a fragrance ingredient in fragrance compounds (mixtures) found 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 provide volume of use of fragrance ingredients for the majority of the fragrance industry.

[1] Calculations were made by Epi Suite (EPA, 2010)

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