



## Review

## Fragrance material review on 3-methyl-2-(pentyloxy)-2-cyclopenten-1-one

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## ABSTRACT

A toxicologic and dermatologic review of 3-methyl-2-(pentyloxy)-2-cyclopenten-1-one when used as a fragrance ingredient is presented. 3-Methyl-2-(pentyloxy)-2-cyclopenten-1-one is a member of the fragrance structural group ketones cyclopentanones and cyclopentenones. The common characteristic structural element of the group members is a cyclopentanone or cyclopentenone ring with a straight or branched chain alkane or alkene substituent. 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 3-methyl-2-(pentyloxy)-2-cyclopenten-1-one were evaluated then summarized and includes physical properties, acute toxicity, skin irritation, mucous membrane (eye) irritation, skin sensitization, phototoxicity, and photoallergy data. A safety assessment of the entire ketones cyclopentanones and cyclopentenones will be published simultaneously with this document; please refer to Belsito et al. (2012) for an overall assessment of the safe use of this material and all ketones cyclopentanones and cyclopentenones in fragrances.

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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 3-methyl-2-(pentyloxy)-2-cyclopenten-1-one (See Fig. 1) when used as a fragrance ingredient. All safety data on 3-methyl-2-(pentyloxy)-2-cyclopenten-1-one were compiled with due diligence including published and unpublished data. In 2008, a complete literature search was conducted on 3-methyl-2-(pentyloxy)-2-cyclopenten-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: 2-Cyclopenten-1-one, 3-methyl-2-(pentyloxy); 2-Cyclopenten-1-one, 2-(pentyloxy)-3-methyl-; 3-Methyl-2-(pentyloxy)cyclopent-2-en-1-one

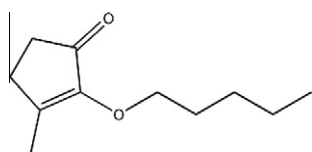


Fig. 1. 3-Methyl-2-(pentyloxy)-2-cyclopenten-1-one.

2.2 CAS registry number: 68922-13-4

2.3 EINECS number: 272-985-7

2.4 Formula: C<sub>11</sub>H<sub>18</sub>O<sub>2</sub>

2.5 Molecular weight: 182.26

## 3. Physical properties

3.1 Boiling point: 268 °C

3.2 Henry's law (calculated): 0.0000578 atm m<sup>3</sup>/mol 25 °C

3.3 Log K<sub>ow</sub> (calculated): 3.01

3.4 Vapor pressure (calculated): 0.00875 mm Hg at 25 °C

3.5 Water solubility (calculated): 144.1 mg/l at 25 °C

3.6 UV spectra available at RIFM; peaks at 240–250 nm and returns to base line at: 340 nm

## 4. Usage

3-Methyl-2-(pentyloxy)-2-cyclopenten-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 3-methyl-2-(pentyloxy)-2-cyclopenten-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 4 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.

### 4.1. Exposure assessment

The dermal systemic exposure in cosmetic products (see Table 1) is calculated based on the concentrations of the same fragrance ingredient in 10 types of the most frequently used personal care and cosmetic products (antiperspirant, bath products, body lotion, eau de toilette, face cream, fragrance cream, hair spray,

Table 1

Calculation of the total human skin exposure from the use of multiple cosmetic products containing 3-methyl-2-(pentyloxy)-2-cyclopenten-1-one.

Product type	Grams applied	Applications per day	Retention factor	Mixture/product (%)	Ingredient/mixture <sup>a</sup>	Ingredient <sup>b</sup> (mg/kg/day)
Antiperspirant	0.5	1	1	0.01	0.01	0.0001
Bath products	17	0.29	0.001	0.02	0.01	0.0000
Body lotion	8	0.71	1	0.004	0.01	0.0004
Eau de toilette	0.75	1	1	0.08	0.01	0.0010
Face cream	0.8	2	1	0.003	0.01	0.0001
Fragrance cream	5	0.29	1	0.04	0.01	0.0010
Hair spray	5	2	0.01	0.005	0.01	0.0000
Shampoo	8	1	0.01	0.005	0.01	0.0000
Shower gel	5	1.07	0.01	0.012	0.01	0.0000
Toilet soap	0.8	6	0.01	0.015	0.01	0.0000
Total						0.0025

<sup>a</sup> Upper 97.5th percentile levels of the fragrance ingredient in the fragrance mixture used in these products.

<sup>b</sup> Based on a 60 kg adult.

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