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Short review

RIFM fragrance ingredient safety assessment, α-Methylbenzyl acetate, CAS Registry Number 93-92-5

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ABSTRACT

The use of this material under current use conditions is supported by the existing information.

This material was evaluated for genotoxicity, repeated dose toxicity, developmental toxicity, reproductive toxicity, local respiratory toxicity, phototoxicity, skin sensitization potential, as well as, environmental safety. Developmental toxicity was determined to have the most conservative systemic exposure derived NO[A]EL of 100 mg/kg/day. A gavage developmental toxicity study conducted in rats on a suitable read across analog resulted in aMOE of 3571 while considering 78.7% absorption from skin contact and 100% from inhalation. A MOE of >100 is deemed acceptable.

1. Identification

1. **Chemical Name:** α-Methylbenzyl acetate
2. **CAS Registry Number:** 93-92-5
3. **Synonyms:** α-Methylbenzyl acetate, Benzenemethanol, α.-methyl-, acetate, Gardenol, Methylphenylcarbinyl acetate, sec-Phenylethyl acetate, α-Phenylethyl acetate, Phenyl methyl carbinyl acetate, Styralyl acetate, ｱﾙｷﾙ(C = 1–5)ｶﾙﾎﾞﾝ酸ﾌｪﾆﾙｱﾙｷﾙ(C = 1–6), 1-Phenylethyl acetate
4. **Molecular Formula:** $C_{10}H_{12}O_2$
5. **Molecular Weight:** 164.2
6. **RIFM Number:** 178

2. Physical data

1. **Boiling Point:** 214 °C [FMA database], 223.12 °C [EPI Suite]
2. **Flash Point:** 195 °F; CC [FMA database]
3. **Log K_{OW}:** 2.5 at 30 °C [RIFM, 1996b], 2.5 [EPI Suite]
4. **Melting Point:** −0.17 °C [EPI Suite]

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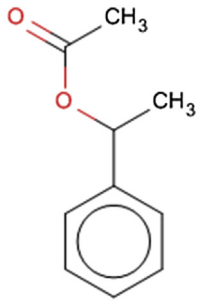
Version: 082415. This version replaces any previous versions.
Name: α-Methylbenzyl acetate
CAS Registry Number: 93-92-5



Abbreviation list:
2-Box Model – a RIFM, Inc. proprietary *in silico* tool used to calculate fragrance air exposure concentration
97.5th **percentile**- The concentration of the fragrance ingredient is obtained from examination of several thousand commercial fine fragrance formulations. The upper 97.5th percentile concentration is calculated from these data and is then used to estimate the dermal systemic exposure in ten types of the most frequently used personal care and cosmetic products. The dermal route is the major route in assessing the safety of fragrance ingredients. Further explanation of how the data were obtained and of how exposures were determined has been previously reported by Cadby et al. (2002) and Ford et al. (2000).
AF- Assessment Factor
BCF- Bioconcentration Factor
DEREK- Derek nexus is an *in silico* tool used to identify structural alerts
DST- Dermal Sensitization Threshold
ECHA-European Chemicals Agency
EU – Europe/European Union
GLP- Good Laboratory Practice
IFRA- The International Fragrance Association
LOEL- Lowest Observable Effect Level
MOE- Margin of Exposure
MPPD - Multiple-Path Particle Dosimetry. An *in silico* model for inhaled vapors used to simulate fragrance lung deposition
NA – North America
NESIL- No Expected Sensitization Induction Level
NOAEC- No Observed Adverse Effect Concentration
NOAEL- No Observed Adverse Effect Level
NOEC- No Observed Effect Concentration
OECD- Organisation for Economic Co-operation and Development
OECD TG- Organisation for Economic Co-operation and Development Testing Guidelines
PBT- Persistent, Bioaccumulative, and Toxic
PEC/PNEC- Predicted Environmental Concentration/Predicted No Effect Concentration
QRA- quantitative risk assessment
REACH- Registration, Evaluation, Authorisation, and Restriction of Chemicals
RIFM- Research Institute for Fragrance Materials
RQ- Risk Quotient
TTC- Threshold of Toxicological Concern
UV/Vis Spectra- Ultra Violet/Visible spectra
VCF- Volatile Compounds in Food
VoU- Volume of Use
vPvB- (very) Persistent, (very) Bioaccumulative
WOE – Weight of Evidences
RIFM's Expert Panel* concludes that this material is safe under the limits described in this safety assessment.
This safety assessment is based on the RIFM Criteria Document (Api et al., 2015) which should be referred to for clarifications.
Each endpoint discussed in this safety assessment reviews the relevant data that were available at the time of writing (version number in the top box is indicative of the date of approval based on a two digit month/day/year), both in the RIFM database (consisting of publicly available and proprietary data) and through publicly available information sources (i.e., SciFinder and PubMed). Studies selected for this safety assessment were based on appropriate test criteria, such as acceptable guidelines, sample size, study duration, route of exposure, relevant animal species, most relevant testing endpoints, etc. A key study for each endpoint was selected based on the most conservative end-point value (e.g., PNEC, NOAEL, LOEL, and NESIL).

5 **Water Solubility:** 481.1 mg/L [EPI Suite]
6 **Specific Gravity:** 1.023–1.026 [FMA database], 1.025–1.028 [FMA], 1.0241 [RIFM Database], 1.03 g/ml [RIFM, 1994], 1.023–1.026 @ 25/25 °C [Gaunt et al., 1974]
7 **Vapor Pressure:** 5.5 Pa at 20 °C [RIFM, 2011], 0.0733 mm Hg @ 20 °C [EPI Suite 4.0], 0.1 mm Hg 20 °C [FMA database], 0.112 mm Hg @ 25 °C [EPI Suite]
8 **UV Spectra:** No significant absorption in the region of 290–700 nm; molar absorption coefficient is below the benchmark (1000 L mol^{-1} cm^{-1}).
9 **Appearance/Organoleptic:** A clear, colorless to pale yellow liquid, having an intense green odor suggesting gardenia.