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2-METHYL-1 PHENYL PROPAN-2-OL: CHEMICO-PHYSICAL DATA, TOXICITY DATA, ENVIRONMENTAL OCCURRENCE AND PERMISSIBLE LEVELS.*

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1. SYNONYMS AND TRADE NAMES

Dimethyl benzyl carbinol, 1,1-dimethyl-2-phenylethanol, α,α-dimethylphenethyl alcohol, benzyl propyl alcohol.

2. CHEMICAL AND PHYSICAL DATA

2.1 Chemical formula

$C_6H_5-CH_2-C(CH_3)_2-OH$ $C_{10}H_{14}O$

2.2 Manufacture

Dimethyl benzyl carbinol is prepared by Grignard synthesis from benzyl magnesium chloride and acetone (Bedoukian, 1967).

2.3 Chemical and physical properties (Food Chem.Codex, 1972)

Appearance	: a white crystalline solid which melts readily; it may exist in supercooled form as a colorless to pale yellow liquid having a floral odour.
Molecular weight	: 150.22
Solubility	: soluble in most fixed oils, in mineral oils and in propylene glycol; it is insoluble in glycerin.

2.4 Typical specifications

	Food Chem.Codex	Givaudan Index
Assay	not less than 97.0%	-
Odour	-	mild floral, woody odour
Colour and appearance	-	colorless to slight yellow liqu at warm room temperature; colou nº 6 max.
Specific gravity (25/25°C)	0.972-0.977	0.971-0.977
Refractive index (20°C) supercooled liquid form	1.514-1.517	1.514-1.518
Solidification point	not less than 22°C	23°C min.
Solubility in alcohol	passes test	clearly soluble in 3 parts of 5 alcohol, 2 parts of 60% alcohol
Limits of impurities: acid value	not more than 1.0	-
Stability and discoloration	-	stable; not known to cause disc loration
Flash point	-	TCC 92.2 °C
Storage		avoid aluminum containers

2.5 Quantitative analysis

No data

3. Uses

Dimethyl benzyl carbinol is used as aromatic agent in fruit flavourings and as fragrance in cosmetics. Levels of use in USA:

	Av.max.ppm
Beverages	3.3
Icecream, ices	3.2
Candy	4
Baked goods	5
Chewing gum	100
Jellies	3.2
Gelatin desserts	0.01
Soap	200-1500
Detergent	20-150
Creams, lotions	100-1000
Perfume	3000-8000

4. METABOLISM

No data

5. TOXICITY DATA

5.1 Acute toxicity

Oral administration of dimethyl benzyl carbinol to rats caused depression and coma; death occurred in 1-24 hr; diuresis and severe gastro-intestinal tract irritation were observed in guinea-pigs and death occurred in 1 hr-4 days (Jenner et al.,1964).

TABLE 1

LD_{50} data of dimethyl benzyl carbinol

Species	Route	LD_{50} (g/kg b.w.)	References
Rat	oral	1.35	Moreno,1973
Rat	oral	1.28	Jenner et al.,1964
Guinea-pig	oral	0.99	Jenner et al.,1964
Rabbit	dermal	5	Moreno,1973

Dimethyl benzyl carbinol applied full strength on intact or abraded rabbit skin was not irritating(Moreno,1973).

5.2 Subacute and subchronic toxicity

In feeding studies in rats, neither 10.000 ppm fed in the diet for 16 weeks, nor 1000 ppm fed in the diet for 28 weeks had any effect on growth or haematology and no macroscopic changes in tissues were observed (Hagan et al.,1967).

5.3 Chronic toxicity and carcinogenicity

No data

5.4 Effects on reproduction

No data

5.5 Mutagenesis studies

No data

6. OBSERVATIONS IN MAN

6.1 Irritation

Dimethyl benzyl carbinol tested at 8% in petrolatum produced no irritation after 48 hr closed-patch test in 25 human subjects (Kligman, 1973).

6.2 Sensitization

A maximization test (Kligman, 1966) was carried out on 25 volunteers; dimethyl benzyl carbinol was tested at concentration of 8% in petrolatum and produced no sensitization reactions (Kligman, 1973).

7. OCCURRENCE

Dimethyl benzyl carbinol has apparently not been reported to occur in nature (Opdyke, 1974).

8. CONCLUSIONS

Dimethyl benzyl carbinol was granted GRAS status by FEMA (1965) and is approved by the FDA for food use (21 CFR 121.1164); the Council of Europe (in press) included dimethyl benzyl carbinol in the list of admissible artificial flavouring substances, at a level of 5 ppm for foods and 3 ppm for beverages.
Further researches are needed particularly in the fields of metabolism, chronic toxicity, carcinogenicity, reproduction and mutagenicity.

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