

TGSC Information System

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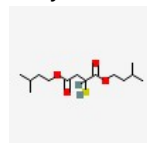
diisopentyl thiomalate

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Name: bis(3-methylbutyl) 2-sulfanylbutanedioate

CAS Number: 68084-03-7



[3D/inchi](#)

ECHA EINECS - REACH Pre-Reg: [268-416-7](#)

FDA UNII: [R38N4Y43EC](#)

Nikkaji Web: [J289.023B](#)

CoE Number: 11454

XlogP3-AA: 3.70 (est)

Molecular Weight: 290.42302000

Formula: C14 H26 O4 S

NMR Predictor: [Predict \(works with chrome, Edge or firefox\)](#)

EFSA/JECFA Comments:

Specifications (EFFA, 2004ak). Racemate (EFFA, 2010a).

Category:flavoring agents

US / EU / FDA / JECFA / FEMA / FLAVIS / Scholar / Patent Information:

Google Scholar: [Search](#)

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JECFA Food Flavoring: [1672 diisopentyl thiomalate](#)

DG SANTE Food Flavorings: [12.108 diisopentyl thiomalate](#)

FEMA Number: [4096](#) diisopentyl thiomalate

FDA: [No longer provide for the use of these seven synthetic flavoring substances](#)

FDA Mainterm (SATF): [68084-03-7 ; DIISOPENTYL THIOMALATE](#)

Physical Properties:

Appearance: pale yellow clear liquid to solid (est)

Assay: 95.00 to 100.00

Additional Assay Information: racemate

Food Chemicals Codex Listed: No

Specific Gravity: 1.01100 to 1.02100 @ 20.00 °C.

Pounds per Gallon - (est): 8.422 to 8.506

Refractive Index: 1.45600 to 1.46000 @ 20.00 °C.

Melting Point: 50.00 °C. @ 760.00 mm Hg

Boiling Point: 140.00 to 155.00 °C. @ 1.00 mm Hg

Boiling Point: 425.00 °C. @ 760.00 mm Hg

Vapor Pressure: 0.000010 mmHg @ 25.00 °C. (est)

Flash Point: > 200.00 °F. TCC (> 93.33 °C.)

logP (o/w): 4.578 (est)

Soluble in:

alcohol

water, 4.789 mg/L @ 25 °C (est)

Insoluble in:

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[Odor type: coffee](#)

Odor Strength: high ,
recommend smelling in a 0.10 % solution or less

Substantivity: 96 hour(s) at 100.00 %

[fermented coffee yeasty bread rye bread](#)

Odor Description: at 0.10 % in dipropylene glycol. fermented coffee yeast dark rye bread

Luebke, William tgsc, (1987)

Odor sample from: PFW Aroma Chemicals

Flavor Type: coffee

[coffee bready yeasty fermented](#)

Taste Description: coffee bready yeasty fermented

Luebke, William tgsc, (1987)

Odor and/or flavor descriptions from others (if found).

Cosmetic Information:

None found

Suppliers:

[BOC Sciences](#)

For experimental / research use only.

[Diisoamyl Thiomalate](#)

[Parchem](#)

[diisoamyl thiomalate](#)

[Penta International](#)

[DIISOAMYL THIOMALATE](#)

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Hazards identification

Classification of the substance or mixture

GHS Classification in accordance with 29 CFR 1910 (OSHA HCS)

None found.

GHS Label elements, including precautionary statements

Pictogram

Hazard statement(s)

None found.

Precautionary statement(s)

None found.

Oral/Parenteral Toxicity:

Not determined

Dermal Toxicity:

Not determined

Inhalation Toxicity:

Not determined

Safety in Use Information:

Category:

flavoring agents

Recommendation for diisoamyl thiomalate usage levels up to:

not for fragrance use.

Maximised Survey-derived Daily Intakes (MSDI-EU): 0.012 (µg/capita/day)