



Formula: C<sub>8</sub>H<sub>14</sub>O<sub>2</sub>S<sub>2</sub>

MW: 206.33

CAS: 1077-28-7

TNP NUMBER: TNP00574

MDL NUMBER: MFCD00005474

IUPAC: 5-(1,2-dithiolan-3-yl)pentanoic acid

Smiles: S1SCCC1CCCC(=O)O

DL-Thioctic acid 98+%, D-form is naturally occurring. Growth factor for many bacteria and protozoa; prosthetic group, coenzyme, or substrates in plants, microorganisms, and animal tissues

THERAPEUTIC CATEGORY: Treatment of liver disease, antidote for poisonous mushrooms.

ACCEPTORS: 2

DONORS: 1

ROTATION BONDS: 6

N+O: 2

Chiral Centers: 1

LogP: 2.98

LogS: -3.64

LIPINSKI: 4

Synonyms: TIMTEC-BB SBB003484;THIOOCTIC ACID;THIOCTIC ACID;(+-)-2-dithiolane-3-pentanoicacid;(+-)-2-dithiolane-3-valericacid;(+/--)-2-dithiolane-3-pentanoicacid;1,2-Dithiolane-3-pentanoicacid,(+-)-(9CI);2-Dithiolane-3-valericacid,(+-)-1

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EINECS:214-071-2

Product Categories:Fatty & Aliphatic Acids, Esters, Alcohols & Derivatives;Substrates;Antioxidant;Biochemistry;Nutritional Supplements;Biochemics;Heterocycles;Sulfur & Selenium Compounds;Food & Flavor Additives;Miscellaneous Compounds DL-Thioctic acid

Chemical Properties: mp 60-62 C bp 160-165 C(lit.) Fp 160-165C storage temp. 2-8C solubility ethanol: 50 mg/mL Water Solubility 0.9 g/L (20 C) Merck 14,9326 BRN 81853 Stability:Stable. Incompatible with strong oxidizing agents.

CAS DataBase Reference: 1077-28-7(

CAS DataBase Reference: ) NIST Chemistry ReferenceDI-thioctic acid(1077-28-7) Xn Risk Statements 22-20/21/22 Safety Statements 37/39-26-24/25-36 WGK Germany 3 RTECS JP1192000 5-(Dithiolan-3-yl)valeric acid DL-Thioctic acid

Usage And Synthesis:

Chemical Properties: Light-Yellow Solid UsageA fat-metabolism stimulator DL-Thioctic acid

