



>>Entry Name: **1,3-Propanedithiol**, 9CI

ENTRY UNDER REVIEW

Synonym(s): 1,3-Dimercaptopropane. Trimethylenedithiol. FEMA 3588

CAS Registry Number: 109-80-8

HSCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>SH

Molecular Formula: C<sub>3</sub>H<sub>8</sub>S<sub>2</sub>

Molecular Weight: 108.228

Accurate Mass: 108.00674

Percentage Composition: C 33.29%; H 7.45%; S 59.26%

Use/Importance: Reagent for prep. of thioketals and thioacetals and demercuration of oxymercury derivs.

Physical Description: Oil

Boiling Point: Bp 169°. Bp<sub>60</sub> 94°

Density: d<sup>20</sup> 1.08

Refractive Index: n<sub>D</sub><sup>20</sup> 1.5405

Aldrich: P5060-9

Fluka: 81800

Sigma: P5266

>>Derivative: Bis-4-methylbenzenesulfonyl

Synonym(s): Trimethylene dithiotosylate

CAS Registry Number: 3866-79-3

Molecular Formula: C<sub>17</sub>H<sub>20</sub>O<sub>4</sub>S<sub>4</sub>

Molecular Weight: 416.607

Accurate Mass: 416.02444

Percentage Composition: C 49.01%; H 4.84%; O 15.36%; S 30.79%

Use/Importance: Reagent for synth. of 1,3-dithianes

Physical Description: Needles (EtOH)

Melting Point: Mp 66-67°

Fluka: 92455

>>Derivative: S,S'-Di-Me

Synonym(s): 1,3-Bis(methylthio)propane, 9CI

CAS Registry Number: 24949-35-7

Molecular Formula: C<sub>5</sub>H<sub>12</sub>S<sub>2</sub>

Molecular Weight: 136.282

Accurate Mass: 136.03804

Percentage Composition: C 44.07%; H 8.87%; S 47.06%

Physical Description: Oil

Boiling Point: Bp<sub>15</sub> 92°

>>Derivative: S,S'-Di-Et

Synonym(s): 1,3-Bis(ethylthio)propane, 9CI

CAS Registry Number: 33672-52-5

Molecular Formula: C<sub>7</sub>H<sub>16</sub>S<sub>2</sub>

Molecular Weight: 164.335

Accurate Mass: 164.06934

Percentage Composition: C 51.16%; H 9.81%; S 39.03%

Physical Description: Oil

Boiling Point: Bp 228-231°. Bp<sub>7</sub> 120°

>>Derivative: S,S'-Di-Ph

Synonym(s): 1,3-Bis(phenylthio)propane

CAS Registry Number: 28118-53-8

Molecular Formula: C<sub>15</sub>H<sub>16</sub>S<sub>2</sub>

Molecular Weight: 260.423

Accurate Mass: 260.06934

Percentage Composition: C 69.18%; H 6.19%; S 24.63%

Boiling Point: Bp<sub>12</sub> 264°