



>>Entry Name: 1-Mercapto-2-propanone, 9CI

Synonym(s): Acetonyl mercaptan. Mercaptoacetone. 2-Oxopropanethiol

CAS Registry Number: 24653-75-6

$\text{H}_3\text{CCOCH}_2\text{SH}$

Molecular Formula: $\text{C}_3\text{H}_6\text{OS}$

Molecular Weight: 90.146

Accurate Mass: 90.013935

Percentage Composition: C 39.97%; H 6.71%; O 17.75%; S 35.57%

Physical Description: Malodorous solid

Melting Point: Mp 112-114° (109-111°)

Other Data: Unstable above 0°

>>Derivative: S-Benzyl

CAS Registry Number: 10230-69-0

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{OS}$

Molecular Weight: 180.27

Accurate Mass: 180.060885

Percentage Composition: C 66.63%; H 6.71%; O 8.88%; S 17.79%

Physical Description: Oil

Boiling Point: Bp₁₇ 155°

Rare Chemicals Library: S64619-9

Other: Oakwood 2509

>>Derivative: S-Ph

>>Derivative: S-(4-Methylphenyl)

Synonym(s): 1-[(4-Methylphenyl)thio]-2-propanone

CAS Registry Number: 1200-13-1

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{OS}$

Molecular Weight: 180.27

Accurate Mass: 180.060885

Percentage Composition: C 66.63%; H 6.71%; O 8.88%; S 17.79%

Physical Description: Oil

Boiling Point: Bp₁₂ 150°

Refractive Index: n_D¹⁸ 1.5642

>>Derivative: S-(4-Methylphenyl), 2,4-dinitrophenylhydrazone

Physical Description: Yellow-orange powder (EtOH)

Melting Point: Mp 114°

>>Derivative: S-(4-Methylphenyl), S-oxide (R-)

Synonym(s): 1-[(4-Methylphenyl)sulfinyl]-2-propanone

CAS Registry Number: 66536-78-5

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{O}_2\text{S}$

Molecular Weight: 196.27

Accurate Mass: 196.0558

Percentage Composition: C 61.20%; H 6.16%; O 16.30%; S 16.34%

Optical Rotation: $[\alpha]_{\text{D}}^{22} +269$ (c, 1 in Me_2CO)

>>Derivative: S-(4-Methylphenyl), S-oxide (S-)

CAS Registry Number: 127583-42-0

Molecular Formula: $\text{C}_{10}\text{H}_{12}\text{O}_2\text{S}$

Molecular Weight: 196.27

Accurate Mass: 196.0558

Percentage Composition: C 61.20%; H 6.16%; O 16.30%; S 16.34%

Optical Rotation: $[\alpha]_{\text{D}}^{22} -269$ (c, 1 in Me_2CO)

>>Derivative: S-(4-Methylphenyl), S-oxide (±)