



>>Entry Name: 4-Mercapto-2-butanone, 8CI

Synonym(s): 2-Thiahexan-5-one

CAS Registry Number: 34619-12-0

HSCH₂CH₂COCH₃

Molecular Formula: C₄H₈OS

Molecular Weight: 104.173

Accurate Mass: 104.029585

Percentage Composition: C 46.12%; H 7.74%; O 15.36%; S 30.78%

Physical Description: Oil

Boiling Point: Bp₁₅ 63-65°

>>Derivative: S-Me

Synonym(s): 4-(Methylthio)-2-butanone, 8CI

CAS Registry Number: 34047-39-7

Molecular Formula: C₅H₁₀OS

Molecular Weight: 118.199

Accurate Mass: 118.045235

Percentage Composition: C 50.81%; H 8.53%; O 13.54%; S 27.13%

Boiling Point: Bp₅₅ 106°. Bp₁₆ 72-73°

Refractive Index: n_D²⁵ 1.4772

Aldrich: W33750-1

Other: Oakwood 2807

>>Derivative: S-Me, 2,4-dinitrophenylhydrazone

Physical Description: Orange prisms (EtOH)

Melting Point: Mp 100.5° (98.5-100°)

>>Derivative: S-Me, semicarbazone

Physical Description: Prisms (CHCl₃/petrol)

Melting Point: Mp 127-128°

>>Derivative: S-Me, S-oxide

Synonym(s): 4-Methylsulfinyl-2-butanone

Molecular Formula: C₅H₁₀O₂S

Molecular Weight: 134.199

Accurate Mass: 134.04015

Percentage Composition: C 44.75%; H 7.51%; O 23.84%; S 23.89%

Physical Description: Cryst. (petrol)

Melting Point: Mp 28-29°

>>Derivative: S-Me, S,S-dioxide

Synonym(s): 4-Methylsulfonyl-2-butanone

CAS Registry Number: 68152-37-4

Molecular Formula: C₅H₁₀O₃S

Molecular Weight: 150.198

Accurate Mass: 150.035065

Percentage Composition: C 39.98%; H 6.71%; O 31.96%; S 21.35%

Physical Description: Cryst. (2-propanol)

Melting Point: Mp 88-89°

>>Derivative: S-Me, S,S-dioxide, oxime

Molecular Formula: C₅H₁₁NO₃S

Molecular Weight: 165.213

Accurate Mass: 165.045964

Percentage Composition: C 36.35%; H 6.71%; N 8.48%; O 29.05%; S 19.41%

Physical Description: Needles (2-propanol)

Melting Point: Mp 107-108°

>>Derivative: S-Et

Synonym(s): 4-(Ethylthio)-2-butanone