



>>Entry Name: 3-Mercapto-2-butanone, 9CI

CAS Registry Number: 40789-98-8

H3CCH(SH)COCH3

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%

Aldrich: W32980-0

>>Variant: (±)-form

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%

>>Derivative: S-Me

Synonym(s): 3-(Methylthio)-2-butanone

CAS Registry Number: 99315-41-0

Extra CAS Registry Numbers(s): 53475-15-3

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: Bp₂₀ 50-54°

Refractive Index: n_D²⁰ 1.4710

>>Derivative: S-Ph

Synonym(s): 3-(Phenylthio)-2-butanone

CAS Registry Number: 13023-53-5

Molecular Formula: C₁₀H₁₂OS

Molecular Weight: 180.27

Accurate Mass: 180.060885

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

Boiling Point: Bp₁₅ 135°

Density: d₄²² 1.077

Refractive Index: n_D²⁰ 1.5550 (1.5563)

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

CAS Registry Number: 35875-07-1

Physical Description: Yellow-orange powder (EtOH)

Melting Point: Mp 101°

References:

Werner, E.G.G., *Rec. Trav. Chim. (J. R. Neth. Chem. Soc.)*, 1949, **68**, 509-519, (*S-Ph*)

Asinger, F. *et al.*, *Annalen*, 1957, **610**, 25, (*synth, S-Me*)

Faller, P. *et al.*, *Bull. Soc. Chim. Fr.*, 1962, 30-34, (*S-Ph*)