



>>Entry Name: 4-Mercapto-4-methyl-2-pentanone, 9CI, 8CI
ENTRY UNDER REVIEW

CAS Registry Number: 19872-52-7



Molecular Formula: $\text{C}_6\text{H}_{12}\text{OS}$

Molecular Weight: 132.226

Accurate Mass: 132.060885

Percentage Composition: C 54.50%; H 9.15%; O 12.10%; S 24.25%

Biological Source: Constit. of *Buxus sempervirens* and *Sarothamnus scoparius*

Physical Description: Liq. with odour of cat urine

Boiling Point: $\text{Bp}_{0.12}$ 55-58°

>>Derivative: S-Ac

Molecular Formula: $\text{C}_8\text{H}_{14}\text{O}_2\text{S}$

Molecular Weight: 174.263

Accurate Mass: 174.07145

Percentage Composition: C 55.14%; H 8.10%; O 18.36%; S 18.40%

Physical Description: Liq.

Boiling Point: Bp_{20} 95°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Cryst. (EtOH or petrol)

Melting Point: Mp 102-103°

>>Derivative: S-Me

Synonym(s): 4-Methyl-4-(methylthio)-2-pentanone. FEMA 3376

CAS Registry Number: 23550-40-5

Molecular Formula: $\text{C}_7\text{H}_{14}\text{OS}$

Molecular Weight: 146.253

Accurate Mass: 146.076535

Percentage Composition: C 57.49%; H 9.65%; O 10.94%; S 21.93%

Boiling Point: Bp_{12} 84°. Bp_{15} 78°

Refractive Index: n_D^{13} 1.4750

References:

Foldi, Z. *et al.*, *J.C.S.*, 1948, 1683, (*synth*)

Asinger, A. *et al.*, *Annalen*, 1957, **610**, 1, (*synth*)

Trost, B.M. *et al.*, *J.A.C.S.*, 1971, **93**, 676, (*synth, nmr, ir*)

Fenaroli's Handbook of Flavor Ingredients, 3rd edn., (ed. Burdock, G.A.), CRC Press, 1995, 573, (*S-Me*)

Encyclopedia of Food and Color Additives, (ed. Burdock, G.A.), CRC Press, 1997, 1871, (*S-Me*)

Tominaga, T. *et al.*, *Flavour Fragrance J.*, 1997, **12**, 373-376, (*isol*)