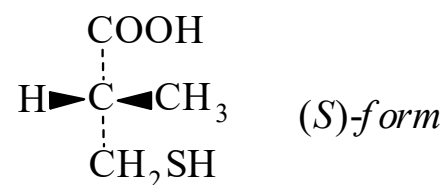




>>Entry Name: 3-Mercapto-2-methylpropanoic acid, 9CI

Synonym(s): β -Mercaptoisobutyric acid



CAS Registry Number: 26473-47-2

Molecular Formula: $\text{C}_4\text{H}_8\text{O}_2\text{S}$

Molecular Weight: 120.172

Accurate Mass: 120.0245

Percentage Composition: C 39.98%; H 6.71%; O 26.63%; S 26.68%

>>Variant: (S)-form

Synonym(s): D-form

CAS Registry Number: 75172-11-1

Molecular Formula: $\text{C}_4\text{H}_8\text{O}_2\text{S}$

Molecular Weight: 120.172

Accurate Mass: 120.0245

Percentage Composition: C 39.98%; H 6.71%; O 26.63%; S 26.68%

Physical Description: Syrup

Boiling Point: Bp_1 62-63°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -27.5$ (c, 2.0 in MeOH)

Refractive Index: n_{D}^{20} 1.4832

>>Derivative: S-Ac

CAS Registry Number: 76497-39-7

Use/Importance: Pharmaceutical intermed.

Physical Description: Oil

Boiling Point: Bp_2 131-132°

Optical Rotation: $[\alpha]_{\text{D}}^{26} -45$ (c, 1.0 in EtOH)

Fluka: 1280

Other: Kaneka D1

>>Variant: ($\pm$)-form

CAS Registry Number: 74709-27-6

Molecular Formula: $\text{C}_4\text{H}_8\text{O}_2\text{S}$

Molecular Weight: 120.172

Accurate Mass: 120.0245

Percentage Composition: C 39.98%; H 6.71%; O 26.63%; S 26.68%

Boiling Point: Bp_{12} 120-122°

>>Derivative: S-Ac

CAS Registry Number: 74407-69-5

Molecular Formula: $\text{C}_6\text{H}_{10}\text{O}_3\text{S}$

Molecular Weight: 162.209

Accurate Mass: 162.035065

Percentage Composition: C 44.43%; H 6.21%; O 29.59%; S 19.77%

Melting Point: Mp 40-40.5°

References:

Larsson, E., *Sven. Kem. Tidskr.*, 1943, **55**, 168; *CA*, **38**, 5798, (*synth*)

Lewis, S.N. *et al.*, *J. Het. Chem.*, 1971, **8**, 571, (*synth*)

Shimazaki, M. *et al.*, *Chem. Pharm. Bull.*, 1982, **30**, 3139, (*synth, abs config*)

Sawayama, T. *et al.*, *Chem. Pharm. Bull.*, 1989, **37**, 1382, (*resoln*)