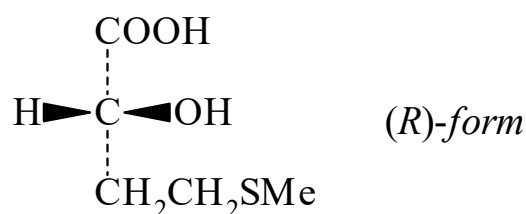




>>Entry Name: 2-Hydroxy-4-(methylthio)butanoic acid

Synonym(s):  $\alpha$ -Hydroxy- $\gamma$ -methylmercaptobutyric acid. Desmeninol, INN. Alimet



CAS Registry Number: 583-91-5

Related CAS Registry Numbers(s): 71597-86-9

Molecular Formula:  $\text{C}_5\text{H}_{10}\text{O}_3\text{S}$

Molecular Weight: 150.198

Accurate Mass: 150.035065

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

>>Variant: (R)-form

CAS Registry Number: 39638-34-1

Extra CAS Registry Numbers(s): 71597-88-1

Molecular Formula:  $\text{C}_5\text{H}_{10}\text{O}_3\text{S}$

Molecular Weight: 150.198

Accurate Mass: 150.035065

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

Physical Description: Oil; cryst. (EtOAc/petrol)(as dicyclohexylamine salt)

Melting Point: Mp 127-129° (dicyclohexylamine salt)

Optical Rotation:  $[\alpha]_{\text{D}}^{25} +22.2$  (c, 1 in EtOH)

>>Variant: (S)-form

CAS Registry Number: 48042-96-2

Molecular Formula:  $\text{C}_5\text{H}_{10}\text{O}_3\text{S}$

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. (as dicyclohexylamine salt)

Melting Point: Mp 128-129° (dicyclohexylamine salt)

Optical Rotation:  $[\alpha]_{\text{D}} -22.5$  (c, 1 in EtOH)

>>Derivative: Et ester

Molecular Formula:  $\text{C}_7\text{H}_{14}\text{O}_3\text{S}$

Molecular Weight: 178.252

Accurate Mass: 178.066365

Percentage Composition: C 47.17%; H 7.92%; O 26.93%; S 17.99%

Optical Rotation:  $[\alpha]_{\text{D}} +20.5$  (c, 1.12 in MeOH)

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

CAS Registry Number: 120-91-2

Molecular Formula:  $\text{C}_5\text{H}_{10}\text{O}_3\text{S}$

Molecular Weight: 150.198

Accurate Mass: 150.035065

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

Use/Importance: Amino acid analogue. Animal and poultry feed additive

Physical Description: Cryst. (as Zn salt)

Melting Point: Mp 250° (Zn salt)

References:

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*Merck Index*, 11th edn., 1989, No. 5897, (use, bibl)

Urban, F.J. *et al.*, *J.O.C.*, 1990, **55**, 3670, (synth, pmr)