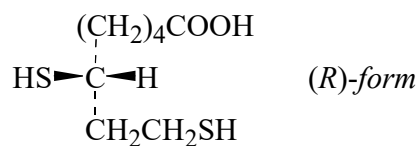




>>Entry Name: 6,8-Dimercaptooctanoic acid, 9CI

Synonym(s): Dihydro- α -lipoic acid



CAS Registry Number: 462-20-4

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_2\text{S}_2$

Molecular Weight: 208.345

Accurate Mass: 208.05917

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

Biological Source: Found in animal and bacterial cells

Use/Importance: Biosynthetic intermed. to α -Lipoic acid [HFD85-X](#)

>>Variant: (R)-form

CAS Registry Number: 119365-69-4

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_2\text{S}_2$

Molecular Weight: 208.345

Accurate Mass: 208.05917

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

Boiling Point: $\text{Bp}_{0.2}$ 145-146°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -10.7$ (c, 1 in EtOH)

>>Variant: (S)-form

CAS Registry Number: 98441-85-1

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_2\text{S}_2$

Molecular Weight: 208.345

Accurate Mass: 208.05917

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

Boiling Point: $\text{Bp}_{0.2}$ 145-146°

Optical Rotation: $[\alpha]_{\text{D}}^{20} +10.7$ (c, 1 in EtOH)

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

CAS Registry Number: 7516-48-5

Molecular Formula: $\text{C}_8\text{H}_{16}\text{O}_2\text{S}_2$

Molecular Weight: 208.345

Accurate Mass: 208.05917

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

Physical Description: Light yellow liq.

Boiling Point: $\text{Bp}_{0.01}$ 170-175° (bath)

>>Derivative: Amide

Synonym(s): Dihydro- α -lipoamide

CAS Registry Number: 4265-09-2

Extra CAS Registry Numbers(s): 3884-47-7

Molecular Formula: $\text{C}_8\text{H}_{17}\text{NOS}_2$

Molecular Weight: 207.36

Accurate Mass: 207.075154

Percentage Composition: C 46.34%; H 8.26%; N 6.75%; O 7.72%; S 30.93%

Physical Description: Cryst.

Melting Point: Mp 66-67°

References:

- Reed, L.J. *et al.*, *J. Biol. Chem.*, 1958, **232**, 143-158, (*synth, amide*)
Reed, L.J. *et al.*, *Acc. Chem. Res.*, 1974, **7**, 40-46, (*rev, biochem*)
Paukstelis, J.V. *et al.*, *J.O.C.*, 1977, **42**, 3941-3944, (*cmr*)
Tsuji, J. *et al.*, *J.O.C.*, 1978, **43**, 3606-3607, (*synth, pmr*)
Pratt, K.J. *et al.*, *Biochem. J.*, 1989, **258**, 749-754, (*synth*)
Ger. Pat., 1993, 4 137 773; *CA*, **119**, 117037j, (*R-from, S-form, synth*)