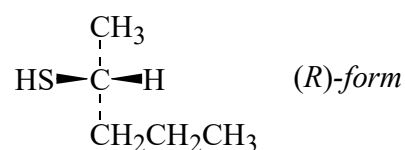




>>Entry Name: 2-Pentanethiol, 9CI

Synonym(s): 2-Mercaptopentane. *sec*-Amyl mercaptan



CAS Registry Number: 2084-19-7

Molecular Formula: C₅H₁₂S

Molecular Weight: 104.216

Accurate Mass: 104.06597

Percentage Composition: C 57.63%; H 11.61%; S 30.77%

>>Variant: (*R*)-form

CAS Registry Number: 212195-83-0

Molecular Formula: C₅H₁₂S

Molecular Weight: 104.216

Accurate Mass: 104.06597

Percentage Composition: C 57.63%; H 11.61%; S 30.77%

Boiling Point: Bp 112°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -4.7$ (c, 17 in Et₂O)

>>Variant: (*S*)-form

CAS Registry Number: 212195-84-1

Molecular Formula: C₅H₁₂S

Molecular Weight: 104.216

Accurate Mass: 104.06597

Percentage Composition: C 57.63%; H 11.61%; S 30.77%

Biological Source: Constit. of the fruit of *Psidium guajava*

Optical Rotation: $[\alpha]_{\text{D}}^{20} +7.9$ (c, 12 in Et₂O)

>>Variant: (±)-form

CAS Registry Number: 110503-18-9

Molecular Formula: C₅H₁₂S

Molecular Weight: 104.216

Accurate Mass: 104.06597

Percentage Composition: C 57.63%; H 11.61%; S 30.77%

Physical Description: Liq.

Boiling Point: Bp 112°

Density: d²⁵ 0.83

Refractive Index: n_D²⁵ 1.4386

Other: PB A31580

>>Derivative: *S*-Me

Synonym(s): 2-(Methylthio)pentane

CAS Registry Number: 13286-91-4

Molecular Formula: C₆H₁₄S

Molecular Weight: 118.243

Accurate Mass: 118.08162

Percentage Composition: C 60.95%; H 11.93%; S 27.12%

Boiling Point: Bp 138.9°. Bp₆₀ 63-64°

Refractive Index: n_D²⁰ 1.4468

>>Derivative: *S*-Me, *S,S*-dioxide

Synonym(s): 2-(Methylsulfonyl)pentane

CAS Registry Number: 101944-72-3

Molecular Formula: C₆H₁₄O₂S

Molecular Weight: 150.241

Accurate Mass: 150.07145

Percentage Composition: C 47.97%; H 9.39%; O 21.30%; S 21.34%

Boiling Point: Bp₂ 101-102°

Refractive Index: n_D²⁰ 1.4602