



>>Entry Name: 6-Mercaptohexanoic acid, 9CI

Synonym(s): 6-Mercaptocaproic acid, 8CI

CAS Registry Number: 17689-17-7

HSCH₂(CH₂)₄COOH

Molecular Formula: C₆H₁₂O₂S

Molecular Weight: 148.226

Accurate Mass: 148.0558

Percentage Composition: C 48.62%; H 8.16%; O 21.59%; S 21.63%

Physical Description: Liq.

Melting Point: Mp 13°

Boiling Point: Bp_{0.8} 112-116°

Refractive Index: n_D²⁵ 1.4811

>>Derivative: Me ester

CAS Registry Number: 20756-86-9

Molecular Formula: C₇H₁₄O₂S

Molecular Weight: 162.252

Accurate Mass: 162.07145

Percentage Composition: C 51.82%; H 8.70%; O 19.72%; S 19.76%

Physical Description: Liq.

Boiling Point: Bp₁ 69°

Refractive Index: n_D²⁶ 1.4629

>>Derivative: Et ester

CAS Registry Number: 101567-75-3

Molecular Formula: C₈H₁₆O₂S

Molecular Weight: 176.279

Accurate Mass: 176.0871

Percentage Composition: C 54.51%; H 9.15%; O 18.15%; S 18.19%

Physical Description: Liq.

Boiling Point: Bp₁₇ 121°. Bp_{0.7} 84-85°

Density: d²⁰ 0.99

Refractive Index: n_D²⁰ 1.4568

>>Derivative: S-Me

Synonym(s): 6-(Methylthio)hexanoic acid, 9CI

CAS Registry Number: 54293-06-0

Molecular Formula: C₇H₁₄O₂S

Molecular Weight: 162.252

Accurate Mass: 162.07145

Percentage Composition: C 51.82%; H 8.70%; O 19.72%; S 19.76%

Physical Description: Oil

>>Derivative: S-Me, S-oxide

Synonym(s): 6-(Methylsulfinyl)hexanoic acid, 9CI

CAS Registry Number: 183858-49-3

Molecular Formula: C₇H₁₄O₃S

Molecular Weight: 178.252

Accurate Mass: 178.066365

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

Physical Description: Cryst.

Melting Point: Mp 48-50°

>>Derivative: S-Me, Me ester

CAS Registry Number: 82921-35-5

Molecular Formula: C₈H₁₆O₂S

Molecular Weight: 176.279

Accurate Mass: 176.0871

Percentage Composition: C 54.51%; H 9.15%; O 18.15%; S 18.19%

Physical Description: Liq.

Boiling Point: Bp₁₅ 117-129°