



>>Entry Name: 3-(Methylthio)propanoic acid, 9CI

ENTRY UNDER REVIEW

CAS Registry Number: 646-01-5

Related CAS Registry Numbers(s): 14090-35-8 71922-81-1

MeSCH₂CH₂COOH

Molecular Formula: C₄H₈O₂S

Molecular Weight: 120.172

Accurate Mass: 120.0245

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

Physical Description: Pale yellow oil or flaky solid (hexane)

Melting Point: Mp 20.5-21.5°

Boiling Point: Bp₁₃ 131-133°

>>Derivative: S,S-Dioxide

Synonym(s): 3-(Methylsulfonyl)propanoic acid, 9CI

CAS Registry Number: 645-83-0

Molecular Formula: C₄H₈O₄S

Molecular Weight: 152.171

Accurate Mass: 152.01433

Percentage Composition: C 31.57%; H 5.30%; O 42.06%; S 21.07%

Physical Description: Cryst. (CHCl₃/Me₂CO)

Melting Point: Mp 102-105°

>>Derivative: Me ester

Synonym(s): FEMA 2720

CAS Registry Number: 13532-18-8

Molecular Formula: C₅H₁₀O₂S

Molecular Weight: 134.199

Accurate Mass: 134.04015

Percentage Composition: C 44.75%; H 7.51%; O 23.84%; S 23.89%

Biological Source: Isol. from pineapple (*Ananas comosus*), melon, naranjila fruit (*Solanum quitonense*) and white wine. Flavouring ingredient

Physical Description: Oil with sweet pineapple flavour at high dilutions

Boiling Point: Bp 170-180°. Bp₁₀₀ 106-108°

Aldrich: 10337-3

Fluka: 67822

>>Derivative: Me ester, S,S-Dioxide

CAS Registry Number: 89211-37-0

Molecular Formula: C₅H₁₀O₄S

Molecular Weight: 166.198

Accurate Mass: 166.02998

Percentage Composition: C 36.13%; H 6.06%; O 38.51%; S 19.29%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 94-94.6°

>>Derivative: Et ester

Synonym(s): FEMA 3343

CAS Registry Number: 13327-56-5

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%

Biological Source: Isol. from pineapple (*Ananas comosus*) and other fruits, also present in alcoholic beverages and Pamesan cheese. Flavouring ingredient

Physical Description: Oil

Boiling Point: Bp₁₈ 88°

Aldrich: W33430-8

>>Derivative: Et ester, S-Oxide, (±)-