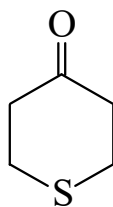




>>Entry Name: Tetrahydro-4*H*-thiopyran-4-one, 9CI

Synonym(s): 4-Thianone. 1-Thia-4-cyclohexanone. Tetrahydrothiopyran-4-one. 4-Oxotetrahydrothiopyran. Tetrahydro-1,4-thiapyrone. Penthianone



CAS Registry Number: 1072-72-6

Molecular Formula: C₅H₈OS

Molecular Weight: 116.184

Accurate Mass: 116.029585

Percentage Composition: C 51.69%; H 6.94%; O 13.77%; S 27.60%

Physical Description: Cryst. (hexane)

Melting Point: Mp 65-66°

Aldrich: 15516-0

Fluka: 87485

Sigma: T6268

>>Derivative: Oxime

CAS Registry Number: 6309-59-7

Molecular Formula: C₅H₉NOS

Molecular Weight: 131.198

Accurate Mass: 131.040484

Percentage Composition: C 45.77%; H 6.91%; N 10.68%; O 12.19%; S 24.44%

Physical Description: Cryst. (EtOH)

Melting Point: Mp 84-86°

>>Derivative: 2,4-Dinitrophenylhydrazone

Physical Description: Cryst. (AcOH)

Melting Point: Mp 186°

>>Derivative: S-Oxide

CAS Registry Number: 17396-36-0

Molecular Formula: C₅H₈O₂S

Molecular Weight: 132.183

Accurate Mass: 132.0245

Percentage Composition: C 45.43%; H 6.10%; O 24.21%; S 24.26%

Physical Description: Cryst. (hexane)

Melting Point: Mp 111-112°

>>Derivative: S,S-Dioxide

CAS Registry Number: 17396-35-9

Molecular Formula: C₅H₈O₃S

Molecular Weight: 148.182

Accurate Mass: 148.019415

Percentage Composition: C 40.53%; H 5.44%; O 32.39%; S 21.64%

Physical Description: Needles (hexane)

Melting Point: Mp 173-174°

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