



>>Entry Name: Thiocarbohydrazide, 8Cl

Synonym(s): Carbonothioic dihydrazide, 9Cl. Thiocarbazide. Thiocarbonic dihydrazide

CAS Registry Number: 2231-57-4

$\text{H}_2\text{NNHCSNHNH}_2$

Molecular Formula: $\text{CH}_6\text{N}_4\text{S}$

Molecular Weight: 106.151

Accurate Mass: 106.031316

Percentage Composition: C 11.31%; H 5.70%; N 52.78%; S 30.21%

Physical Description: Cryst. (H_2O)

Other Data: Dec. at 170°

Hazard & Toxicity: LD_{50} (mus, ipr) 5 mg/kg

Aldrich: 22322-0

Fluka: 88535

Rare Chemicals Library: S54845-6

Sigma: T2137

>>Derivative: 1,5-Di-Ac

Molecular Formula: $\text{C}_5\text{H}_{10}\text{N}_4\text{O}_2\text{S}$

Molecular Weight: 190.226

Accurate Mass: 190.052446

Percentage Composition: C 31.57%; H 5.30%; N 29.45%; O 16.82%; S 16.86%

Physical Description: Hygroscopic cryst.

Melting Point: Mp $204\text{--}205^\circ$

>>Derivative: 1-Ph

CAS Registry Number: 2550-71-2

Molecular Formula: $\text{C}_7\text{H}_{10}\text{N}_4\text{S}$

Molecular Weight: 182.249

Accurate Mass: 182.062616

Percentage Composition: C 46.13%; H 5.53%; N 30.74%; S 17.59%

Physical Description: Tablets (EtOH)

Solubility: Sol. EtOH , AcOH , Py; spar. sol. Me_2CO , CHCl_3 , C_6H_6

>>Derivative: 1-Ph; hydrochloride

Physical Description: Plates

Melting Point: Mp 181°

>>Derivative: 1-Me, 1-Ph

Molecular Formula: $\text{C}_8\text{H}_{12}\text{N}_4\text{S}$

Molecular Weight: 196.276

Accurate Mass: 196.078266

Percentage Composition: C 48.96%; H 6.16%; N 28.54%; S 16.34%

Physical Description: Prisms (EtOH)

Melting Point: Mp $228\text{--}229$ dec. $^\circ$

>>Derivative: Di-Ph

References:

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 805B, (ir)

Guha, P.C. *et al.*, *J.C.S.*, 1924, 1215, (synth)

Burns, G.R., *Inorg. Chem.*, 1968, **7**, 277, (synth)

Braibanti, A. *et al.*, *J.C.S. Perkin 2*, 1972, 2116, (cryst struct)

Gowda, B. *et al.*, *Proc. Indian Acad. Sci., Chem. Sci.*, 1990, **102**, 463, (synth)

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