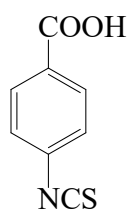




>>Entry Name: 4-Isothiocyanatobenzoic acid, 9CI

Synonym(s): 4-Carboxyphenyl isothiocyanate



CAS Registry Number: 2131-62-6

Molecular Formula: $C_8H_5NO_2S$

Molecular Weight: 179.199

Accurate Mass: 179.004099

Percentage Composition: C 53.62%; H 2.81%; N 7.82%; O 17.86%; S 17.89%

Physical Description: Cryst. (Me_2CO)

Melting Point: Mp 220°

>>Derivative: Et ester

CAS Registry Number: 1205-06-7

Molecular Formula: $C_{10}H_9NO_2S$

Molecular Weight: 207.253

Accurate Mass: 207.035399

Percentage Composition: C 57.95%; H 4.38%; N 6.76%; O 15.44%; S 15.47%

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 58° (56.5°)

Other Data: A Mp of 98° may also occur in the lit.; this appears to be erroneous

>>Derivative: Chloride

CAS Registry Number: 53611-24-8

Molecular Formula: C_8H_4ClNOS

Molecular Weight: 197.644

Accurate Mass: 196.970211

Percentage Composition: C 48.62%; H 2.04%; Cl 17.94%; N 7.09%; O 8.10%; S 16.22%

Physical Description: Cryst.

Melting Point: Mp 75°

Boiling Point: Bp₂ 130-140°

>>Derivative: Anhydride

CAS Registry Number: 110409-17-1

Molecular Formula: $C_{16}H_8N_2O_3S_2$

Molecular Weight: 340.383

Accurate Mass: 339.997633

Percentage Composition: C 56.46%; H 2.37%; N 8.23%; O 14.10%; S 18.84%

Physical Description: Yellow cryst. (C_6H_6)

Melting Point: Mp 215-216°

References:

Dyson, G.M., *J.C.S.*, 1927, 436, (*Et ester, synth*)

Browne, D.W. *et al.*, *J.C.S.*, 1934, 178, (*synth, esters*)

Sayigh, A.A.R. *et al.*, *J.O.C.*, 1965, **30**, 2465, (*Et ester, synth, pmr*)

Kricheldorf, H.R., *Makromol. Chem.*, 1973, **167**, 1, (*synth*)

Viswanathan, N. *et al.*, *Indian J. Chem., Sect. B*, 1981, **20**, 308, (*chloride*)

Eur. Pat., 1987, 220 899; *CA*, **107**, 130518p, (*anhydride, synth, pmr*)

Wilcox, C.S. *et al.*, *Tetrahedron*, 1995, **51**, 621, (*Et ester, synth, pmr, cmr, ir*)