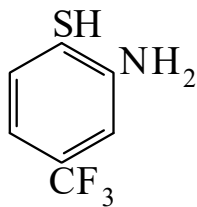




>>Entry Name: 2-Amino-4-(trifluoromethyl)benzenethiol, 9Cl, 8Cl

Synonym(s): 2-Mercapto-5-(trifluoromethyl)aniline



CAS Registry Number: 19406-49-6

Related CAS Registry Numbers(s): 368-75-2

Molecular Formula: C₇H₆F₃NS

Molecular Weight: 193.192

Accurate Mass: 193.017303

Percentage Composition: C 43.52%; H 3.13%; F 29.50%; N 7.25%; S 16.60%

Physical Description: Oil

Boiling Point: Bp₂ 77-78°

Refractive Index: n_D²⁵ 1.5332

>>Derivative: Hydrochloride

CAS Registry Number: 4274-38-8

Physical Description: Cryst. (EtOH/HCl)

Melting Point: Mp 196-198 dec.°

Aldrich: 36573-4

>>Derivative: S-Me

Molecular Formula: C₈H₈F₃NS

Molecular Weight: 207.219

Accurate Mass: 207.032953

Percentage Composition: C 46.37%; H 3.89%; F 27.50%; N 6.76%; S 15.47%

Boiling Point: Bp₁₂ 112°

References:

Dannley, R.L. *et al.*, *Can. J. Chem.*, 1965, **43**, 2610, (*synth, derivs*)

Palmer, P.J. *et al.*, *J. Med. Chem.*, 1971, **14**, 248, (*synth*)

Mylari, B.L. *et al.*, *J. Med. Chem.*, 1991, **34**, 108, (*synth, pmr, ms*)