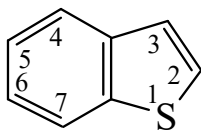




>>Entry Name: Benzo[*b*]thiophene, 9CI

Synonym(s): Thianaphthene. Benzothiofuran. 1-Thiaindene. Thionaphthene



CAS Registry Number: 95-15-8

Related CAS Registry Numbers(s): 51500-42-6

Extra CAS Registry Numbers(s): 11095-43-5

Molecular Formula: C₈H₆S

Molecular Weight: 134.201

Accurate Mass: 134.01902

Percentage Composition: C 71.60%; H 4.51%; S 23.89%

Source/Synthesis: Present in coal tars

Physical Description: Leaflets with naphthalene odour

Melting Point: Mp 32°

Boiling Point: Bp 221-222°. Bp₂₀ 103-105°

Other Data: Steam-volatile

Aldrich: T2740-5

Fluka: 12808

>>Derivative: Picrate

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 149°

>>Derivative: S,S-Dioxide

CAS Registry Number: 825-44-5

Molecular Formula: C₈H₆O₂S

Molecular Weight: 166.2

Accurate Mass: 166.00885

Percentage Composition: C 57.81%; H 3.64%; O 19.25%; S 19.29%

Melting Point: Mp 142-143°

Rare Chemicals Library: S85241-4

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **3**, 174A, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 685A, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1506C, (*ir*)
Porter, Q.N., *Aust. J. Chem.*, 1967, **20**, 103, (*ms*)
Iddon, B. *et al.*, *Adv. Heterocycl. Chem.*, 1970, **11**, 177, (*rev*)
Balkau, F. *et al.*, *Aust. J. Chem.*, 1972, **25**, 327, (*pmr*)
Barrault, J. *et al.*, *J. Chem. Res., Synop.*, 1978, 207, (*synth*)
Wudl, F. *et al.*, *J.O.C.*, 1979, **44**, 2491, (*uv*)
Geneste, P. *et al.*, *J.O.C.*, 1979, **44**, 2887, (*cmr*)
Scrowston, R.M. *et al.*, *Adv. Heterocycl. Chem.*, 1981, **28**, 1503, (*rev*)
Al-Showiman, S.S. *et al.*, *Org. Magn. Reson.*, 1982, **20**, 105, (*cmr*)
El Faghi, M.S. *et al.*, *Acta Cryst. C*, 1987, **43**, 2421, (*cryst struct, dioxide*)
Kitamura, T. *et al.*, *Chem. Lett.*, 1988, 1637, (*synth*)
McKillop, A. *et al.*, *Tetrahedron*, 1989, **45**, 3299, (*synth, dioxide*)
Russavskaya, N.V. *et al.*, *J. Org. Chem. USSR (Engl. Transl.)*, 1990, **26**, 587, (*synth*)
Kreher, R.P. *et al.*, *Chem. Ber.*, 1991, **124**, 645, (*bibl*)
Rozen, S. *et al.*, *Chem. Comm.*, 1994, 1959, (*dioxide*)