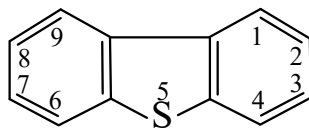




>>Entry Name: **Dibenzothiophene**, 9CI, USAN
Synonym(s): Diphenylene sulfide. 9-Thiafluorene



CAS Registry Number: 132-65-0

Molecular Formula: C₁₂H₈S
Molecular Weight: 184.261
Accurate Mass: 184.03467
Percentage Composition: C 78.22%; H 4.38%; S 17.40%
Use/Importance: Keratolytic agent
Physical Description: Cryst. (petrol)
Melting Point: Mp 99°
Boiling Point: Bp 332-333°. Bp₃ 152-154°
Calculated Log P Data: Log P 4.56 (calc)

Aldrich: 34783-3
Fluka: 42990
Supelco: R42-3050

>>Derivative: Picrate

Physical Description: Yellow cryst. (EtOH)
Melting Point: Mp 125°

>>Derivative: S-Oxide

CAS Registry Number: 1013-23-6
Molecular Formula: C₁₂H₈OS
Molecular Weight: 200.261
Accurate Mass: 200.029585
Percentage Composition: C 71.97%; H 4.03%; O 7.99%; S 16.01%
Melting Point: Mp 189.5-190° (183-185°)
Rare Chemicals Library: S81803-8

>>Derivative: S,S-Dioxide

CAS Registry Number: 1016-05-3
Molecular Formula: C₁₂H₈O₂S
Molecular Weight: 216.26
Accurate Mass: 216.0245
Percentage Composition: C 66.65%; H 3.73%; O 14.80%; S 14.83%
Physical Description: Cryst. (EtOH)
Melting Point: Mp 230°
Aldrich: D3240-7

References:

- Aldrich Library of ¹³C and ¹H FT NMR Spectra*, 1992, **3**, 174B; 174C, (*nmr*)
Aldrich Library of FT-IR Spectra, 1st edn., 1985, **2**, 685B; 685C, (*ir*)
Aldrich Library of FT-IR Spectra: Vapor Phase, 1989, **3**, 1506D, (*ir*)
Rahman, A.U. *et al.*, *Tet. Lett.*, 1968, 3925, (*synth*)
Schaffrin, R.M. *et al.*, *J.C.S.(A)*, 1970, 1561, (*cryst struct*)
Bartle, K.D. *et al.*, *Tetrahedron*, 1971, **27**, 5177, (*pmr*)
Ashby, J. *et al.*, *Adv. Heterocycl. Chem.*, 1974, **16**, 181, (*rev*)
Benati, L. *et al.*, *Gazz. Chim. Ital.*, 1975, **105**, 841, (*synth*)
Giraud, J. *et al.*, *Org. Magn. Reson.*, 1979, **12**, 647, (*cmr*)
Riepe, W. *et al.*, *Org. Mass Spectrom.*, 1979, **14**, 455, (*ms*)
Dunkerton, L.V. *et al.*, *J. Het. Chem.*, 1987, **24**, 749, (*cmr*)