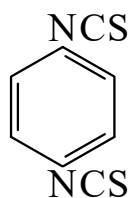




>>Entry Name: 1,4-Diisothiocyanatobenzene, 9CI

Synonym(s): *p*-Phenylene isothiocyanate, 8CI. Phenylene-1,4-diisothiocyanate. **Bitoscanate**, INN. Biscomate. Jonit. Yonit. Hoe 16842. WM 842. DITC



CAS Registry Number: 4044-65-9

Type of Compound Code(s): XA0900

Molecular Formula: C₈H₄N₂S₂

Molecular Weight: 192.265

Accurate Mass: 191.981588

Percentage Composition: C 49.98%; H 2.10%; N 14.57%; S 33.36%

Source/Synthesis: Manuf. from 1,4-benzenediamine, CS₂ and NH₃

Use/Importance: Anthelmintic. Coupling reagent for solid-phase synthesis and sequencing of proteins

Physical Description: Needles (Me₂CO)

Melting Point: Mp 132°

Calculated Log P Data: Log P 5.19 (calc)

Other Data: Forms high molecular-weight polymers with dihydrazides

Hazard & Toxicity: LD₅₀ (mus, orl) 230 mg/kg

Aldrich: 25855-5

Fluka: 78480

Sigma: P0158

References:

- Aldrich Library of 13C and 1H FT NMR Spectra*, 1992, **2**, 1555A, (*nmr*)
Pohloudek-Fabini, R. *et al.*, *Arch. Pharm. (Weinheim, Ger.)*, 1960, **292**, 666, (*synth*)
Lieber, E. *et al.*, *J.O.C.*, 1962, **27**, 2214, (*synth*)
Kristian, P. *et al.*, *Coll. Czech. Chem. Comm.*, 1965, **30**, 3658, (*synth, ir*)
Christ, O. *et al.*, *Arzneim.-Forsch.*, 1970, **20**, 756, (*metab*)
Jucker, E., *Prog. Drug Res.*, (Ed.), 1975, **19**, 2, (*rev, pharmacol*)
Liang, S.-P. *et al.*, *Anal. Biochem.*, 1980, **188**, 366; 1991, **197**, 163, (*use*)
Laursen, R.A. *et al.*, *Methods Biochem. Anal.*, 1980, **26**, 201, (*use, rev*)
Daniei, I. *et al.*, *Chem. Zvesti*, 1984, **38**, 539, (*cmr*)
Katritzky, A.R. *et al.*, *J. Polym. Sci., Part A: Polym. Chem.*, 1987, **25**, 311, (*polymers*)
Martindale, The Extra Pharmacopoeia, 30th edn., *Pharmaceutical Press*, 1993, 40
Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., *Van Nostrand Reinhold*, 1992, PFA500