



>>Entry Name: 4,4'-Diaminodiphenyl ether

Synonym(s): 4,4'-Oxybisbenzenamine, 9Cl. 4,4'-Oxydianiline, 8Cl. Bis(4-aminophenyl) ether

CAS Registry Number: 101-80-4

Molecular Formula: C₁₂H₁₂N₂O

Molecular Weight: 200.24

Accurate Mass: 200.094963

Percentage Composition: C 71.98%; H 6.04%; N 13.99%; O 7.99%

Use/Importance: Cross-linking agent for polymers

Melting Point: Mp 186-187°

pKa Value: pK_a 5.21 (50% EtOH aq.)

Hazard & Toxicity: Possible human carcinogen. LD₅₀ (rat, orl) 725 mg/kg. Exp. carcinogen and teratogen

Aldrich: A7250-2

Fluka: 32930

Sigma: A8158

References:

Aldrich Library of 13C and 1H FT NMR Spectra, 1992, **2**, 485A, (nmr)

Aldrich Library of FT-IR Spectra, 1st edn., 1985, **1**, 1210A, (ir)

Reynolds, G.A. *et al.*, *J.A.C.S.*, 1951, **73**, 4996, (synth)

Shamis, E.M. *et al.*, *J. Org. Chem. USSR (Engl. Transl.)*, 1967, **3**, 1005, (synth)

Frankovskii, C.S. *et al.*, *J. Org. Chem. USSR (Engl. Transl.)*, 1970, **6**, 2305, (uv)

Dzhioev, F.K., *CA*, 1975, **83**, 73149d, (tox)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials, 8th edn.*, Van Nostrand Reinhold, 1992, OPM000