



>>Entry Name: 4,4'-Dinitrodiphenyl sulfide

Synonym(s): 1,1'-Thiobis(4-nitrobenzene), 9Cl. Bis(*p*-nitrophenyl) sulfide, 8Cl. Di(4-nitrophenyl) sulfide

CAS Registry Number: 1223-31-0

Structure by analogy with 2,2'-Dinitrodiphenyl sulfide, [FBG33-X](#)

Molecular Formula: C₁₂H₈N₂O₄S

Molecular Weight: 276.272

Accurate Mass: 276.020478

Percentage Composition: C 52.17%; H 2.92%; N 10.14%; O 23.16%; S 11.61%

Physical Description: Orange plates (AcOH)

Melting Point: Mp 156-157°

Hazard & Toxicity: LD₅₀ (rat, orl) 1490 mg/kg

Rare Chemicals Library: S65879-0

>>Derivative: S,S-Dioxide

Synonym(s): 4,4'-Dinitrodiphenyl sulfone. 1,1'-Sulfonylbis[4-nitrobenzene], 9Cl. Bis(*p*-nitrophenyl) sulfone, 8Cl. Di(4-nitrophenyl) sulfone

CAS Registry Number: 1156-50-9

Molecular Formula: C₁₂H₈N₂O₆S

Molecular Weight: 308.271

Accurate Mass: 308.010308

Percentage Composition: C 46.75%; H 2.62%; N 9.09%; O 31.14%; S 10.40%

Physical Description: Cryst. (AcOH)

Melting Point: Mp 282°

References:

Cole, E.R., *Chem. Ind. (London)*, 1957, 1511, (*synth, dioxide*)

Chi, Y.-L. *et al.*, *CA*, 1959, **53**, 18896, (*dioxide*)

Castrillon, J.P.A. *et al.*, *J.O.C.*, 1965, **30**, 1338

Vowinkel, E. *et al.*, *Chem. Ber.*, 1974, **107**, 898, (*synth*)

Martin, G.E. *et al.*, *J. Het. Chem.*, 1978, **15**, 609, (*cmr*)

Huang, X. *et al.*, *Synthesis*, 1986, 967, (*synth*)

Lewis, R.J., *Sax's Dangerous Properties of Industrial Materials*, 8th edn., Van Nostrand Reinhold, 1992, BLA750