



>>Entry Name: 1-Nitro-4-(phenylthio)benzene, 9Cl

Synonym(s): 4-Nitrodiphenyl sulfide. *p*-Nitrophenyl phenyl sulfide, 8Cl

CAS Registry Number: 952-97-6

Molecular Formula: C₁₂H₉NO₂S

Molecular Weight: 231.275

Accurate Mass: 231.035399

Percentage Composition: C 62.32%; H 3.92%; N 6.06%; O 13.84%; S 13.86%

Physical Description: Yellow prisms (petrol)

Melting Point: Mp 55°

Boiling Point: Bp₁₀₀ 288.2°. Bp₂₅ 240°

Rare Chemicals Library: S46100-8

>>Derivative: *S*-Oxide, (±)-form

Synonym(s): 4-Nitrodiphenyl sulfoxide. 1-Nitro-4-(phenylsulfinyl)benzene, 9Cl. *p*-Nitrophenyl phenyl sulfone

CAS Registry Number: 955-45-3

Molecular Formula: C₁₂H₉NO₃S

Molecular Weight: 247.274

Accurate Mass: 247.030314

Percentage Composition: C 58.29%; H 3.67%; N 5.66%; O 19.41%; S 12.97%

Melting Point: Mp 107-107.5°

>>Derivative: *S,S*-Dioxide

Synonym(s): 4-Nitrodiphenyl sulfone. 1-Nitro-4-(phenylsulfonyl)benzene, 9Cl. *p*-Nitrophenyl phenyl sulfone, 8Cl

CAS Registry Number: 1146-39-0

Molecular Formula: C₁₂H₉NO₄S

Molecular Weight: 263.273

Accurate Mass: 263.025229

Percentage Composition: C 54.75%; H 3.45%; N 5.32%; O 24.31%; S 12.18%

Physical Description: Needles (EtOH aq.)

Melting Point: Mp 143°

Rare Chemicals Library: S79996-3

References:

Szmant, H.H. *et al.*, *J.A.C.S.*, 1951, **73**, 4356, (*synth, uv, oxide*)

Kornblum, N. *et al.*, *J.O.C.*, 1976, **41**, 1560, (*synth*)

Ando, W. *et al.*, *Tet. Lett.*, 1982, **23**, 1685, (*oxide*)

Pettrillo, G. *et al.*, *Tet. Lett.*, 1985, **20**, 6365, (*synth*)

Morley, J. *et al.*, *J.C.S. Perkin 2*, 1987, 1361, (*uv*)

Chandrasekaran, R. *et al.*, *Magn. Reson. Chem.*, 1987, **25**, 1001; 1989, **27**, 360, (*pmr, cmr, oxide*)

Compton, R.G. *et al.*, *J.C.S. Perkin 2*, 1995, 1673, (*oxide, dioxide*)