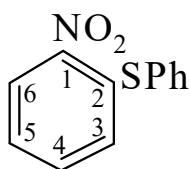




>>Entry Name: 1-Nitro-2-(phenylthio)benzene, 9CI

Synonym(s): *o*-Nitrophenyl phenyl sulfide, 8CI. 2-Nitrodiphenyl sulfide



CAS Registry Number: 4171-83-9

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 needles (petrol)

Melting Point: Mp 80.2°

Aldrich: 46899-1

>>Derivative: *S*-Oxide, (±)-form

CAS Registry Number: 18739-95-2

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%

Physical Description: Yellow needles (petrol)

Melting Point: Mp 92-93°

>>Derivative: *S,S*-Dioxide

Synonym(s): 1-Nitro-2-(phenylsulfonyl)benzene, 9CI. 2-Nitrodiphenyl sulfone. *o*-Nitrophenyl phenyl sulfone

CAS Registry Number: 31515-43-2

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%

Biological Use/Importance: Shows anti-HIV activity

Physical Description: Cryst. (EtOH)

Melting Point: Mp 147.5°

Aldrich: 46900-9

Rare Chemicals Library: S91934-9

References:

- Leandri, G. *et al.*, *J.C.S.*, 1957, 1386, (*synth, uv, oxide*)
Kornblum, N. *et al.*, *J.O.C.*, 1976, **41**, 1560-1564, (*synth*)
Gillis, R., *Aust. J. Chem.*, 1990, **43**, 1779, (*ms*)
Balicky, R. *et al.*, *Annalen*, 1992, 883, (*synth, oxide*)