



>>Entry Name: 1-(Methylthio)-4-nitrobenzene, 9CI

Synonym(s): Methyl *p*-nitrophenyl sulfide, 8CI. *p*-Nitrothioanisole. 1-Methylmercapto-4-nitrobenzene

CAS Registry Number: 701-57-5

Related CAS Registry Numbers(s): 940-12-5 112456-63-0

Molecular Formula: C₇H₇NO₂S

Molecular Weight: 169.204

Accurate Mass: 169.019749

Percentage Composition: C 49.69%; H 4.17%; N 8.28%; O 18.91%; S 18.95%

Physical Description: Yellow leaflets (petrol), plates (MeOH)

Melting Point: Mp 72-73°

Boiling Point: Bp₂ 132°

Aldrich: 29186-2

>>Derivative: *S*-Oxide

Synonym(s): Methyl 4-nitrophenyl sulfoxide

CAS Registry Number: 940-12-5

Molecular Formula: C₇H₇NO₃S

Molecular Weight: 185.203

Accurate Mass: 185.014664

Percentage Composition: C 45.40%; H 3.81%; N 7.56%; O 25.92%; S 17.31%

Melting Point: Mp 151-152°

>>Derivative: *S*-Oxide (*R*-)

Synonym(s): 1-(Methylsulfinyl)-4-nitrobenzene, 9CI

CAS Registry Number: 93222-06-1

Molecular Formula: C₇H₇NO₃S

Molecular Weight: 185.203

Accurate Mass: 185.014664

Percentage Composition: C 45.40%; H 3.81%; N 7.56%; O 25.92%; S 17.31%

Physical Description: Solid

Melting Point: Mp 150.4-152.6°

Optical Rotation: [α]_D +156.9 (c, 0.75 in CHCl₃) (99.3% ee)

Other Data: Mp quoted here is for (*S*)-isomer with ee = 55%

>>Derivative: *S,S*-Dioxide

Synonym(s): 1-(Methylsulfonyl)-4-nitrobenzene, 9CI

CAS Registry Number: 2976-30-9

Molecular Formula: C₇H₇NO₄S

Molecular Weight: 201.203

Accurate Mass: 201.009579

Percentage Composition: C 41.79%; H 3.51%; N 6.96%; O 31.81%; S 15.94%

Physical Description: Needles (AcOH or EtOH)

Melting Point: Mp 142.5° (136°)

References:

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Jeminet, G. *et al.*, *Bull. Soc. Chim. Fr.*, 1967, 3233, (*synth*)
Biffen, M.E.C. *et al.*, *Aust. J. Chem.*, 1974, **27**, 777, (*synth*)
Dai, L.-X. *et al.*, *Synth. Commun.*, 1994, **24**, 2229, (*oxide, synth*)
Nagata, T. *et al.*, *Bull. Chem. Soc. Jpn.*, 1995, **68**, 3241, (*S-oxide, synth, pmr, ir*)
Compton, R.G. *et al.*, *J.C.S. Perkin 2*, 1995, 1673, (*sulfoxide, sulfone synth, pmr*)
Brunel, J.-M. *et al.*, *J.O.C.*, 1995, **60**, 8086, (*S-oxide, synth, ir, pmr*)