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Typical Product Specifications & Properties

1-(Methylsulfonyl)-3-Nitrobenzene

CAS Number: : 2976-32-1

Specifications	Limits
SMILES	[N+](=[O-])(=O)c1cc(S(=O)(=O)C)ccc1
InChI	FTJMAAWQEAOBBI-UHFFFAOYSA-N
InChIKey	1S/C7H7NO4S/c1-13(11,12)7-4-2-3-6(5-7)8(9)10/h2-5H,1H3
log P (octanol-water)	0.5
Vapor Pressure	3.39E-05 mm Hg
Water solubility	6580 mg/L
Atmospheric OH Rate Constant	1.11E-12 cm ³ /molecule-sec
Henry's Law Constant	4.92E-09 atm-m ³ /mole



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