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Typical Product Specifications & Properties

3-Nitro-N-(3-Nitrophenyl)Benzamide

CAS Number: : 101-24-6

Specifications	Limits
Molecular weight	287.23
EINECS	202-927-8
SMILES	<chem>O=C(Nc1cccc([N+])([O-])=O)c1)c1cccc([N+])([O-])=O)c1</chem>
InChI	IGYJMXLXTJJVRS-UHFFFAOYSA-N
InChIKey	1S/C13H9N3O5/c17-13(9-3-1-5-11(7-9)15(18)19)14-10-4-2-6-12(8-10)16(20)21/h1-8H,(H,14,17)
Molecular weight	258.10
EINECS	202-930-4
SMILES	<chem>c1(cc(ccc1)Cl)NC(OCC#CCCl)=O</chem>
InChI	1S/C11H9Cl2NO2/c12-6-1-2-7-16-11(15)14-10-5-3-4-9(13)8-10/h3-5,8H,6-7H2,(H,14,15)
InChIKey	MCOQHIWZJUDQIC-UHFFFAOYSA-N
Boiling Point	224 dec ° C
Atmospheric OH Rate Constant	5.54E-11 cm ³ /molecule-sec



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Specifications	Limits
Henry's Law Constant	1.17E-08 atm-m ³ /mole
Vapor Pressure	3.80E-07 mm Hg
Melting Point	75 ° C
log P (octanol-water)	3.410
Water solubility	11 mg/L



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