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Typical Product Specifications & Properties

1,2-Di-Tert-Butylbenzene

CAS Number: : 1012-76-6

Specifications	Limits
Molecular weight	190.32
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 cm3/molecule-sec
Henry's Law Constant	1.17E-08 atm-m3/mole
Vapor Pressure	3.80E-07 mm Hg
Melting Point	75 ° C
log P (octanol-water)	3.410



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Specifications	Limits
Water solubility	11 mg/L
Molecular weight	275.52
EINECS	202-910-5
SMILES	<chem>c1(Nc2c(cccc2)Cl)nc(nc(n1)Cl)Cl</chem>
InChI	1S/C9H5Cl3N4/c10-5-3-1-2-4-6(5)13-9-15-7(11)14-8(12)16-9/h1-4H,(H,13,14,15,16)
InChIKey	IMHBYKMAHXWHRP-UHFFFAOYSA-N
log P (octanol-water)	3.88
Water solubility	8 mg/L
Atmospheric OH Rate Constant	4.28E-11 cm ³ /molecule-sec
Vapor Pressure	6.20E-09 mm Hg
Henry's Law Constant	2.81E-10 atm-m ³ /mole
Melting Point	160 °C



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Specifications	Limits
Molecular weight	186.17
EINECS	202-928-3
SMILES	<chem>O=NN1CN2CN(CN(C2)N=O)C1</chem>
Specifications	Limits
InChI	1S/C5H10N6O2/c12-6-10-2-8-1-9(4-10)5-11(3-8)7-13/h1-5H2
InChIKey	MWRWFPQBGSZ WNV-UHFFFAOYSA-N
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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