

Typical Product Specifications & Properties

5-Chlorobenzotriazole

CAS Number: : 39994-75-9

Specifications	Limits
Molecular weight	394.42
EINECS	201-501-9
SMILES	<chem>c1c2c(O[C@H](C3)C(=C)C)ccc1C(=O)[C@@H]1[C@H](O2)COc2c1cc(c(c2)OC)OC</chem>
InChI	1S/C23H22O6/c1-11(2)16-8-14-15(28-16)6-5-12-22(24)21-13-7-18(25-3)19(26-4)9-17(13)27-10-20(21)29-23(12)14/h5-7,9,16,20-21H,1,8,10H2,2-4H3
InChIKey	JUVIOZPCNVVQFO-UHFFFAOYSA-N
Water solubility	0.2 mg/L
log P (octanol-water)	4.1
Atmospheric OH Rate Constant	3.29E-10 cm ³ /molecule-sec
Henry's Law Constant	1.12E-13 atm-m ³ /mole
Melting Point	176 °C