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Typical Product Specifications & Properties

4-Bromo-3-nitroaniline

CAS Number: : 53324-38-2

Specifications	Limits
Molecular weight	217.02
InChI	1S/C6H5BrN2O2/c7-5-2-1-4(8)3-6(5)9(10)11/h1-3H,8H2
InChIKey	PITHQPMZWKZGRZ-UHFFFAOYSA-N
Molecular weight	450.98
EINECS	251-443-3
SMILES	Cl.COc1ccc(cc1)[C@@H]2Sc3ccccc3N(CCN(C)C)C(=O)[C@@H]2OC(=O)C
InChI	HDRXZJPWHTXQRI-BHDTVMLSSA-N
InChIKey	1S/C22H26N2O4S.ClH/c1-15(25)28-20-21(16-9-11-17(27-4)12-10-16)29-19-8-6-5-7-18(19)24(22(20)26)14-13-23(2)3;/h5-12,20-21H,13-14H2,1-4H3;1H/t20-,21+;/m1./s1
Melting Point	207.5-212 ° C
log P (octanol-water)	2.7
Water solubility	12.3 mg/L
Henry's Law Constant	8.61E-17 atm-m ³ /mole



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Specifications	Limits
Atmospheric OH Rate Constant	1.80E-10 cm ³ /molecule-sec
Vapor Pressure	1.54E-11 mm Hg
Storage Temperature	2-8°C
Flash Point	2?
Melting Point	212-214 °C
Merck	13,3226
Refractive Index	118 ° (C=1, H ₂ O)
Water solubility	soluble
Color	White to off-white
Flash Point	2?
Form	Powder



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