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Typical Product Specifications & Properties

3-Fluorobenzoic Acid

CAS Number: : 455-38-9

Specifications	Limits
Molecular weight	140.11
EINECS	207-248-0
SMILES	<chem>c1(cc(ccc1)F)C(O)=O</chem>
InChI	1S/C7H5FO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,(H,9,10)
InChIKey	MXNBDFWNYRNIBH-UHFFFAOYSA-N
Density	1.474
BRN Number	1906920
Storage Temperature	Refrigerator
Melting Point	122-124 °C
Water solubility	Very soluble in water.
Atmospheric OH Rate Constant	1.19E-12 cm ³ /molecule-sec
log P (octanol-water)	2.15



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Specifications	Limits
pKa Dissociation Constant	3.86
Vapor Pressure	0.059 mm Hg
Water solubility	1500 mg/L
Melting Point	124 ° C
Henry's Law Constant	1.27E-07 atm-m ³ /mole



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