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Typical Product Specifications & Properties

2-Chloro-5-nitrobenzoic Acid

CAS Number: : 2516-96-3

Specifications	Limits
Molecular weight	201.56
SMILES	<chem>c1(cc(ccc1Cl)[N+](=O)[O-])C(O)=O</chem>
InChI	1S/C7H4ClNO4/c8-6-2-1-4(9(12)13)3-5(6)7(10)11/h1-3H,(H,10,11)
InChIKey	QUEKGYQTRJVEQC-UHFFFAOYSA-N
Water solubility	3600 mg/L
Henry's Law Constant	3.17E-10 atm-m ³ /mole
Vapor Pressure	1.89E-05 mm Hg
Atmospheric OH Rate Constant	5.83E-13 cm ³ /molecule-sec
pKa Dissociation Constant	2.17
Melting Point	166.5 °C
log P (octanol-water)	2.03



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415 Huguenot Street, New Rochelle, New York 10801

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