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Typical Product Specifications & Properties

2-Chloro-4-nitrobenzoic acid

CAS Number: : 99-60-5

Specifications	Limits
Molecular weight	201.56
EINECS	202-771-0
SMILES	<chem>c1(cc(c(C(=O)=O)cc1)Cl)[N+](=O)[O-]</chem>
InChI	QAYNSPOKTRVZRC-UHFFFAOYSA-N
InChIKey	1S/C7H4ClNO4/c8-6-3-4(9(12)13)1-2-5(6)7(10)11/h1-3H,(H,10,11)
log P (octanol-water)	2.03
Atmospheric OH Rate Constant	5.64E-13 cm ³ /molecule-sec
Melting Point	140 ° C
Henry's Law Constant	3.17E-10 atm-m ³ /mole
Water solubility	323 mg/L
pKa Dissociation Constant	2.14
Vapor Pressure	1.89E-05 mm Hg



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Specifications	Limits
Melting Point	136-140 °C
Water solubility	1 g/L (20 °C)
BRN Number	1912836



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