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Typical Product Specifications & Properties

3-Aminobenzoic acid

CAS Number: : 99-05-8

Specifications	Limits
Molecular weight	137.14
EINECS	202-724-4
SMILES	<chem>Nc1cc(cc(c1)C(=O)O</chem>
InChI	1S/C7H7NO2/c8-6-3-1-2-5(4-6)7(9)10/h1-4H,8H2,(H,9,10)
InChIKey	XFDUHJPVQKIXHO-UHFFFAOYSA-N
Atmospheric OH Rate Constant	2.99E-11 cm ³ /molecule-sec
pKa Dissociation Constant	3.07
Water solubility	5900 mg/L
Vapor Pressure	2.78E-04 mm Hg
Henry's Law Constant	3.83E-11 atm-m ³ /mole
Melting Point	173 °C
log P (octanol-water)	0.65



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415 Huguenot Street, New Rochelle, New York 10801

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