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Typical Product Specifications & Properties

2-Chloro-6-methylbenzoic acid

CAS Number: : 21327-86-6

Specifications	Limits
Molecular weight	170.59
SMILES	<chem>OC(=O)c1c(Cl)cccc1C</chem>
InChI	CEFMMQYDPGICYMG-UHFFFAOYSA-N
InChIKey	1S/C8H7ClO2/c1-5-3-2-4-6(9)7(5)8(10)11/h2-4H,1H3,(H,10,11)
Water solubility	651 mg/L
pKa Dissociation Constant	2.75
log P (octanol-water)	2.31
Atmospheric OH Rate Constant	1.98E-12 cm ³ /molecule-sec
Vapor Pressure	8.86E-04 mm Hg
Henry's Law Constant	8.87E-08 atm-m ³ /mole
Melting Point	103-105°C
BRN Number	2614092

