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Typical Product Specifications & Properties

3-Cyanobenzoic acid

CAS Number: : 1877-72-1

Specifications	Limits
Molecular weight	147.13
EINECS	217-511-1
SMILES	<chem>c1(cc(ccc1)C#N)C(O)=O</chem>
InChI	1S/C8H5NO2/c9-5-6-2-1-3-7(4-6)8(10)11/h1-4H,(H,10,11)
InChIKey	GYLKKXHEIIFTJH-UHFFFAOYSA-N
Water solubility	2310 mg/L
log P (octanol-water)	1.48
Melting Point	219 ° C
Atmospheric OH Rate Constant	6.47E-13 cm ³ /molecule-sec
pKa Dissociation Constant	3.6
Vapor Pressure	2.09E-04 mm Hg
Henry's Law Constant	1.05E-09 atm-m ³ /mole



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Specifications	Limits
Storage Temperature	Store at room temperature.
Melting Point	220-224 °C
BRN Number	1862566



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