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Typical Product Specifications & Properties

4,6-Dimethylnicotinic Acid

CAS Number: : 22047-86-5

Specifications	Limits
Molecular weight	151.16
Molecular weight	198.13
EINECS	208-601-1
SMILES	<chem>c1(cc(cc(c1O)C)[N+](=O)[O-])[N+](=O)[O-]</chem>
InChI	1S/C7H6N2O5/c1-4-2-5(8(11)12)3-6(7(4)10)9(13)14/h2-3,10H,1H3
InChIKey	ZXVONLUNISGICL-UHFFFAOYSA-N
Henry's Law Constant	1.40E-06 atm-m ³ /mole
Vapor Pressure	1.06E-04 mm Hg
Boiling Point	378 ° C
Melting Point	86.6 ° C
Water solubility	198 mg/L
Atmospheric OH Rate Constant	3.03E-13 cm ³ /molecule-sec



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Specifications	Limits
pKa Dissociation Constant	4.31
log P (octanol-water)	2.12
Storage Temperature	0-6°C
Flash Point	11 °C
Boiling Point	196°C 1012mm
Melting Point	83-85 °C
Water solubility	slightly soluble
Merck	3279



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