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Typical Product Specifications & Properties

3-Methylisoxazole-5-carboxylic acid

CAS Number: : 4857-42-5

Specifications	Limits
Molecular weight	127.10
EINECS	225-454-9
SMILES	<chem>Cc1cc(no1)C(=O)O</chem>
InChI	BNMPIJWVMVNSRD-UHFFFAOYSA-N
InChIKey	1S/C5H5NO3/c1-3-2-4(5(7)8)6-9-3/h2H,1H3,(H,7,8)
pKa Dissociation Constant	2.2
Atmospheric OH Rate Constant	7.14E-12 cm ³ /molecule-sec
log P (octanol-water)	0.68
Water solubility	2.48E+04 mg/L
Henry's Law Constant	1.26E-09 atm-m ³ /mole
Vapor Pressure	0.015 mm Hg



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