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Typical Product Specifications & Properties

(3-nitrophenoxy)acetic acid

CAS Number: : 1878-88-2

Specifications	Limits
Molecular weight	197.14
EINECS	217-528-4
SMILES	<chem>OC(=O)COc1cccc(c1)[N+](=O)[O-]</chem>
InChI	BNRRQAASFDGMMQ-UHFFFAOYSA-N
InChIKey	1S/C8H7NO5/c10-8(11)5-14-7-3-1-2-6(4-7)9(12)13/h1-4H,5H2,(H,10,11)
Vapor Pressure	1.42E-05 mm Hg
Henry's Law Constant	6.62E-11 atm-m3/mole
pKa Dissociation Constant	2.95
Atmospheric OH Rate Constant	6.67E-12 cm3/molecule-sec
Water solubility	3090 mg/L
log P (octanol-water)	1.37



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415 Huguenot Street, New Rochelle, New York 10801

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