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Typical Product Specifications & Properties

Nitrilotriacetic acid

CAS Number: : 139-13-9

Specifications	Limits
Molecular weight	191.14
EINECS	205-355-7
SMILES	<chem>N(CC(O)=O)(CC(O)=O)CC(O)=O</chem>
InChI	1S/C6H9NO6/c8-4(9)1-7(2-5(10)11)3-6(12)13/h1-3H2,(H,8,9)(H,10,11)(H,12,13)
InChIKey	MGFYIUFZLHCRTH-UHFFFAOYSA-N
Henry's Law Constant	1.30E-10 atm-m3/mole
Melting Point	242 dec ° C
log P (octanol-water)	-3.810
Atmospheric OH Rate Constant	7.90E-11 cm3/molecule-sec
Vapor Pressure	7.00E-09 mm Hg
Water solubility	5.91E+04 mg/L
pKa Dissociation Constant	3.03



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Specifications	Limits
Melting Point	245 °C (dec.)
Water solubility	Insoluble.<0.01 g/100 mL at 23 ºC
Flash Point	100 °C
Storage Temperature	Store at room temperature.
Merck	14,6579
Solubility	0.1 M NaOH: 0.1 M at 20 °C, clear, colorless



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