

Typical Product Specifications & Properties

2-Nitroisophthalic Acid

CAS Number: : 21161-11-5

Specifications	Limits
Molecular weight	211.13
EINECS	244-253-7
SMILES	<chem>[N+](=O)([O-])c1c(cccc1C(=O)O)C(=O)O</chem>
InChI	CAHWDGJDQYAFHM-UHFFFAOYSA-N
InChIKey	1S/C8H5NO6/c10-7(11)4-2-1-3-5(8(12)13)6(4)9(14)15/h1-3H,(H,10,11)(H,12,13)
log P (octanol-water)	0.890
Atmospheric OH Rate Constant	1.06E-12 cm ³ /molecule-sec
Water solubility	2160 mg/L