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## Typical Product Specifications & Properties

# Metsulphuron-Methyl

CAS Number: : 74223-64-6

Specifications	Limits
Molecular weight	381.37
SMILES	<chem>c1(c(ccc1)C(=O)OC)S(=O)(=O)NC(=O)Nc1nc(nc(n1)C)OC</chem>
InChI	RSMUVYRMZCOLBH-UHFFFAOYSA-N
InChIKey	1S/C14H15N5O6S/c1-8-15-12(18-14(16-8)25-3)17-13(21)19-26(22,23)10-7-5-4-6-9(10)11(20)24-2/h4-7H,1-3H3,(H2,15,16,17,18,19,21)
Storage Temperature	0-6&deg;C
Melting Point	158&deg;C
Melting Point	158 &deg; C
Henry's Law Constant	1.32E-16 atm-m <sup>3</sup> /mole
pKa Dissociation Constant	3.64
Water solubility	9500 mg/L
Atmospheric OH Rate Constant	2.52E-11 cm <sup>3</sup> /molecule-sec
log P (octanol-water)	2.2



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Specifications	Limits
Molecular weight	224.15
SMILES	<chem>P(O\C(=C\C(OC)=O)C)(OC)(OC)=O</chem>
InChI	1S/C7H13O6P/c1-6(5-7(8)10-2)13-14(9,11-3)12-4/h5H,1-4H3/b6-5+
InChIKey	GEPDYQSQVLXLEU-AATRIKPKSA-N
log P (octanol-water)	0.13
Vapor Pressure	1.28E-04 mm Hg
Melting Point	13.95 &deg; C
Henry's Law Constant	6.39E-11 atm-m <sup>3</sup> /mole
Water solubility	6.00E+05 mg/L
Atmospheric OH Rate Constant	3.63E-11 cm <sup>3</sup> /molecule-sec



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