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Typical Product Specifications & Properties

Demeton

CAS Number: : 8065-48-3

Specifications	Limits
Molecular weight	516.68
SMILES	<chem>P(=O)(OCC)(OCC)SCCSCC.P(=S)(OCC)(OCC)OCCSCC</chem>
InChI	1S/2C8H19O3PS2/c1-4-10-12(9,11-5-2)14-8-7-13-6-3;1-4-9-12(13,10-5-2)11-7-8-14-6-3/h2*4-8H2,1-3H3
InChIKey	FAXIJTUDSBIMHY-UHFFFAOYSA-N
Water solubility	666 mg/L
Vapor Pressure	1.30E-03 mm Hg
Henry's Law Constant	3.82E-06 atm-m3/mole
Atmospheric OH Rate Constant	1.33E-10 cm3/molecule-sec
log P (octanol-water)	3.210
Molecular weight	330.36
EINECS	204-497-7
InChI	1S/C10H19O6PS2/c1-5-15-9(11)7-8(10(12)16-6-2)19-17(18,13-3)14-4/h8H,5-7H2,1-4H3



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Specifications	Limits
InChIKey	JXSJBGJIGXNWCI-UHFFFAOYSA-N
Atmospheric OH Rate Constant	7.74E-11 cm ³ /molecule-sec
Henry's Law Constant	4.89E-09 atm-m ³ /mole
Melting Point	2.8 ° C
Vapor Pressure	3.38E-06 mm Hg
log P (octanol-water)	2.36
Water solubility	143 mg/L
Water solubility	0.0145 g/100 mL
Stability	Stable. Incompatible with oxidizing agents, metals.
Flash Point	-18 °C
Density	1.2076
Boiling Point	156°C



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Specifications	Limits
Storage Temperature	APPROX 4°C
Melting Point	2.85°C
Molecular weight	323.30
Specifications	Limits
EINECS	218-276-8
SMILES	<chem>c1([P@@](Oc2ccc([N+](=O)[O-])cc2)(OCC)=S)ccccc1</chem>
InChI	1S/C14H14NO4PS/c1-2-18-20(21,14-6-4-3-5-7-14)19-13-10-8-12(9-11-13)15(16)17/h3-11H,2H2,1H3
InChIKey	AIGRXSNSLVJMEA-UHFFFAOYSA-N
Water solubility	3.11 mg/L
Melting Point	36 ° C
Henry's Law Constant	4.44E-07 atm-m3/mole
Atmospheric OH Rate Constant	7.47E-11 cm3/molecule-sec
log P (octanol-water)	4.78



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Specifications	Limits
Vapor Pressure	9.50E-07 mm Hg
Molecular weight	224.15
EINECS	232-095-1
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-AATRICKPKSA-N
log P (octanol-water)	0.13
Vapor Pressure	1.28E-04 mm Hg
Melting Point	13.95 ° C
Henry's Law Constant	6.39E-11 atm-m ³ /mole
Water solubility	6.00E+05 mg/L
Atmospheric OH Rate Constant	3.63E-11 cm ³ /molecule-sec



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Specifications	Limits
Molecular weight	456.54
EINECS	201-107-7
SMILES	<chem>P(=S)(SC1C(SP(=S)(OCC)OCC)OCCO1)(OCC)OCC</chem>
InChI	1S/C12H26O6P2S4/c1-5-15-19(21,16-6-2)23-11-12(14-10-9-13-11)24-20(22,17-7-3)18-8-4/h11-12H,5-10H2,1-4H3
InChIKey	VBKKVDGJXVOLNE-UHFFFAOYSA-N
Atmospheric OH Rate Constant	7.94E-10 cm ³ /molecule-sec
Vapor Pressure	8.76E-08 mm Hg
log P (octanol-water)	3.450
Henry's Law Constant	1.35E-11 atm-m ³ /mole
Melting Point	-2.00E+01 ° C
Specifications	Limits
Water solubility	1.550 mg/L



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