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Typical Product Specifications & Properties

Pipracil

CAS Number: : 61477-96-1

Specifications	Limits
Molecular weight	517.55
EINECS	262-811-8
SMILES	<chem>CCN1CCN(C(=O)C1=O)C(=O)N[C@H](c2ccccc2)C(=O)N[C@H]3[C@@H]4N(C3=O)[C@H](C(S4)(C)C)C(=O)O</chem>
InChI	IVBHGBMCVLDMKU-GXNBUGAJSA-N
InChIKey	1S/C23H27N5O7S/c1-4-26-10-11-27(19(32)18(26)31)22(35)25-13(12-8-6-5-7-9-12)16(29)24-14-17(30)28-15(21(33)34)23(2,3)36-20(14)28/h5-9,13-15,20H,4,10-11H2,1-3H3,(H,24,29)(H,25,35)(H,33,34)/t13-,14-,15+,20-/m1/s1
Water solubility	207 mg/L
Vapor Pressure	2.47E-22 mm Hg
Atmospheric OH Rate Constant	1.05E-10 cm ³ /molecule-sec
Henry's Law Constant	2.62E-30 atm-m ³ /mole
log P (octanol-water)	0.5
Melting Point	183-185°C (dec.)
RTECS	XH8952200



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Specifications	Limits
Storage Temperature	Hygroscopic, -20°C Freezer, Under Inert Atmosphere
Solubility	Freely soluble in methanol. Only sparingly soluble in aqueous solution at 0.119 mg/mL



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