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Typical Product Specifications & Properties

Chlorazepate Dipotassium

CAS Number: : 57109-90-7

Specifications	Limits
Molecular weight	408.92
EINECS	260-565-6
SMILES	[K+].O[K]. [O-]C(=O)C1N=C(c2ccccc2)c3cc(Cl)ccc3NC1=O
InChI	QCHSEDTUUKDTIG-UHFFFAOYSA-L
InChIKey	1S/C16H11ClN2O3.2K.H2O/c17-10-6-7-12-11(8-10)13(9-4-2-1-3-5-9)19-14(16(21)22)15(20)18-12;;;/h1-8,14H,(H,18,20)(H,21,22);;;1H2/q;2*+1;/p-2
Molecular weight	299.76
EINECS	200-371-0
SMILES	CNC1=Nc2ccc(cc2C(=[N+](C1)[O-])c3ccccc3)Cl
InChI	1S/C16H14ClN3O/c1-18-15-10-20(21)16(11-5-3-2-4-6-11)13-9-12(17)7-8-14(13)19-15/h2-9H,10H2,1H3,(H,18,19)
InChIKey	ANTSCNMPPGJYLG-UHFFFAOYSA-N
Melting Point	236.2 ° C
log P (octanol-water)	2.44



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Specifications	Limits
Vapor Pressure	1.03E-11 mm Hg
Water solubility	2000 mg/L
Henry's Law Constant	4.24E-17 atm-m3/mole
pKa Dissociation Constant	4.8
Atmospheric OH Rate Constant	8.26E-11 cm3/molecule-sec
Storage Temperature	Controlled Substance, -20°C Freezer, Under Inert Atmosphere
Flash Point	9?
Melting Point	230-232°C



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