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Typical Product Specifications & Properties

1H-1,5-Benzodiazepine-2,4(3H,5H)-dione, 7-chloro-1-methyl-5-phenyl-

CAS Number: : 22316-47-8

Specifications	Limits
Molecular weight	300.74
EINECS	244-908-7
SMILES	<chem>c12N(c3ccccc3)C(=O)CC(=O)N(c1ccc(c2)Cl)C</chem>
InChI	CXOXHMZGEKVPMU-UHFFFAOYSA-N
InChIKey	1S/C16H13ClN2O2/c1-18-13-8-7-11(17)9-14(13)19(16(21)10-15(18)20)12-5-3-2-4-6-12/h2-9H,10H2,1H3
Henry's Law Constant	2.91E-10 atm-m ³ /mole
Atmospheric OH Rate Constant	1.81E-11 cm ³ /molecule-sec
log P (octanol-water)	2.12
Water solubility	188 mg/L
Vapor Pressure	7.33E-10 mm Hg



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