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Typical Product Specifications & Properties

C06817

CAS Number: : 28981-97-7

Specifications	Limits
Molecular weight	308.77
EINECS	249-349-2
SMILES	<chem>c12c(C(c3ccccc3)=NCc3n1c(nn3)C)cc(Cl)cc2</chem>
InChI	1S/C17H13ClN4/c1-11-20-21-16-10-19-17(12-5-3-2-4-6-12)14-9-13(18)7-8-15(14)22(11)16/h2-9H,10H2,1H3
InChIKey	VREFGVBLTWBCJP-UHFFFAOYSA-N
Vapor Pressure	1.65E-08 mm Hg
Water solubility	13.1 mg/L
Atmospheric OH Rate Constant	7.62E-12 cm ³ /molecule-sec
Henry's Law Constant	9.77E-12 atm-m ³ /mole
log P (octanol-water)	2.12
Storage Temperature	2-8°C
Flash Point	11 °C



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Specifications	Limits
Solubility	H2O: insoluble
Melting Point	228-228.50C



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