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Typical Product Specifications & Properties

1,3-dihydro-5-phenyl-2H-1,4-benzodiazepin-2-one

CAS Number: : 2898-08-0

Specifications	Limits
Molecular weight	236.27
EINECS	220-781-3
SMILES	<chem>c1ccc(cc1)C2=NCC(=O)Nc3c2ccccc3</chem>
InChI	IVUAAOBNUNMJQC-UHFFFAOYSA-N
InChIKey	1S/C15H12N2O/c18-14-10-16-15(11-6-2-1-3-7-11)12-8-4-5-9-13(12)17-14/h1-9H,10H2,(H,17,18)
Storage Temperature	Store at -15°C
log P (octanol-water)	2.18
Vapor Pressure	2.36E-08 mm Hg
Henry's Law Constant	2.40E-10 atm-m ³ /mole
Atmospheric OH Rate Constant	1.99E-11 cm ³ /molecule-sec
Water solubility	387 mg/L



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