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Typical Product Specifications & Properties

Desmedipham

CAS Number: : 13684-56-5

Specifications	Limits
Molecular weight	300.31
SMILES	<chem>c1c(OC(Nc2ccccc2)=O)cccc1NC(OCC)=O</chem>
InChI	1S/C16H16N2O4/c1-2-21-15(19)18-13-9-6-10-14(11-13)22-16(20)17-12-7-4-3-5-8-12/h3-11H,2H2,1H3,(H,17,20)(H,18,19)
InChIKey	WZJZMXBKUWKXTQ-UHFFFAOYSA-N
Henry's Law Constant	1.69E-10 atm-m ³ /mole
Melting Point	120 ° C
log P (octanol-water)	3.39
Atmospheric OH Rate Constant	9.13E-11 cm ³ /molecule-sec
Vapor Pressure	3.00E-09 mm Hg
pKa Dissociation Constant	12.9
Water solubility	7 mg/L



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