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Typical Product Specifications & Properties

Phenmedipham

CAS Number: : 13684-63-4

Specifications	Limits
Molecular weight	300.31
EINECS	237-199-0
SMILES	<chem>Cc1cccc(c1)NC(=O)Oc2cccc(c2)NC(=O)OC</chem>
InChI	1S/C16H16N2O4/c1-11-5-3-6-12(9-11)18-16(20)22-14-8-4-7-13(10-14)17-15(19)21-2/h3-10H,1-2H3,(H,17,19)(H,18,20)
InChIKey	IDOWTHOLJBTAFI-UHFFFAOYSA-N
Water solubility	<0.1 g/100 mL at 2
Storage Temperature	0-6°C
Melting Point	140-144°C
Flash Point	100 °C
Henry's Law Constant	8.41E-13 atm-m3/mole
Atmospheric OH Rate Constant	1.91E-10 cm3/molecule-sec
log P (octanol-water)	3.59



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Specifications	Limits
Water solubility	4.7 mg/L
pKa Dissociation Constant	0.1
Vapor Pressure	1.00E-11 mm Hg
Melting Point	143 ° C



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