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Typical Product Specifications & Properties

Sigmodal

CAS Number: : 1216-40-6

Specifications	Limits
Molecular weight	317.18
SMILES	<chem>CCCC(C)C1(CC(=C)Br)C(=O)NC(=O)NC1=O</chem>
InChI	1S/C12H17BrN2O3/c1-4-5-7(2)12(6-8(3)13)9(16)14-11(18)15-10(12)17/h7H,3-6H2,1-2H3,(H2,14,15,16,17,18)
InChIKey	ZGVCLZRQOUEZHG-UHFFFAOYSA-N
Water solubility	160 mg/L
log P (octanol-water)	2.09
Vapor Pressure	8.23E-13 mm Hg
Atmospheric OH Rate Constant	3.12E-11 cm ³ /molecule-sec
Henry's Law Constant	1.66E-13 atm-m ³ /mole



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415 Huguenot Street, New Rochelle, New York 10801

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