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Typical Product Specifications & Properties

Talbutal

CAS Number: : 115-44-6

Specifications	Limits
Molecular weight	224.26
SMILES	<chem>CCC(C)C1(CC=C)C(=O)NC(=O)NC1=O</chem>
InChI	1S/C11H16N2O3/c1-4-6-11(7(3)5-2)8(14)12-10(16)13-9(11)15/h4,7H,1,5-6H2,2-3H3,(H2,12,13,14,15,16)
InChIKey	BJVVMKUXKQHWJK-UHFFFAOYSA-N
Henry's Law Constant	6.29E-13 atm-m3/mole
Melting Point	109 ° C
Vapor Pressure	2.31E-11 mm Hg
Atmospheric OH Rate Constant	4.27E-11 cm3/molecule-sec
pKa Dissociation Constant	7.79
log P (octanol-water)	1.47
Water solubility	1810 mg/L



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415 Huguenot Street, New Rochelle, New York 10801

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