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Typical Product Specifications & Properties

Butalbital, USP

CAS Number: : 77-26-9

Specifications	Limits
Molecular weight	224.26
EINECS	201-017-8
SMILES	<chem>C1(C(NC(=O)NC1=O)=O)(CC(C)C)CC=C</chem>
InChI	1S/C11H16N2O3/c1-4-5-11(6-7(2)3)8(14)12-10(16)13-9(11)15/h4,7H,1,5-6H2,2-3H3,(H2,12,13,14,15,16)
InChIKey	UZVHFVZFNXBMQJ-UHFFFAOYSA-N
log P (octanol-water)	1.870
Water solubility	1700 mg/L
Atmospheric OH Rate Constant	3.91E-11 cm ³ /molecule-sec
Melting Point	138.5 °C



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415 Huguenot Street, New Rochelle, New York 10801

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