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Typical Product Specifications & Properties

Narcobarbital

CAS Number: : 125-55-3

Specifications	Limits
Molecular weight	303.15
SMILES	<chem>CC(C)C1(CC(=C)Br)C(=O)NC(=O)N(C)C1=O</chem>
InChI	1S/C11H15BrN2O3/c1-6(2)11(5-7(3)12)8(15)13-10(17)14(4)9(11)16/h6H,3,5H2,1-2,4H3,(H,13,15,17)
InChIKey	WGMAVSHOSNKMF-UHFFFAOYSA-N
log P (octanol-water)	2.11
Water solubility	186 mg/L
Henry's Law Constant	2.07E-13 atm-m ³ /mole
Melting Point	115 ° C
Atmospheric OH Rate Constant	2.75E-11 cm ³ /molecule-sec
Vapor Pressure	2.03E-11 mm Hg