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Typical Product Specifications & Properties

Secobarbital

CAS Number: : 76-73-3

Specifications	Limits
Molecular weight	238.28
EINECS	200-982-2
SMILES	<chem>C1(C(NC(=O)NC1=O)=O)([C@@H](CCC)C)CC=C</chem>
InChI	1S/C12H18N2O3/c1-4-6-8(3)12(7-5-2)9(15)13-11(17)14-10(12)16/h5,8H,2,4,6-7H2,1,3H3,(H2,13,14,15,16,17)
InChIKey	KQPKPCNLIDLUMF-UHFFFAOYSA-N
log P (octanol-water)	1.97
pKa Dissociation Constant	7.8
Atmospheric OH Rate Constant	4.41E-11 cm ³ /molecule-sec
Henry's Law Constant	8.35E-13 atm-m ³ /mole
Vapor Pressure	3.36E-10 mm Hg
Melting Point	100 ° C
Water solubility	550 mg/L



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