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Typical Product Specifications & Properties

C Carrie

CAS Number: : 50-36-2

Specifications	Limits
Molecular weight	303.35
EINECS	200-032-7
SMILES	CN1[C@H]2CC[C@@H]1[C@H]([C@H](C2)OC(=O)c3ccccc3)C(=O)OC
InChI	ZPUCINDJVBVPJ-LJISPDSOSA-N
InChIKey	1S/C17H21NO4/c1-18-12-8-9-13(18)15(17(20)21-2)14(10-12)22-16(19)11-6-4-3-5-7-11/h3-7,12-15H,8-10H2,1-2H3/t12-,13+,14-,15+/m0/s1
log P (octanol-water)	2.3
pKa Dissociation Constant	8.61
Water solubility	1800 mg/L
Vapor Pressure	1.91E-07 mm Hg
Melting Point	98 ° C
Henry's Law Constant	4.24E-11 atm-m ³ /mole
Atmospheric OH Rate Constant	5.30E-11 cm ³ /molecule-sec



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