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Typical Product Specifications & Properties

Phenesterin

CAS Number: : 3546-10-9

Specifications	Limits
Molecular weight	644.81
SMILES	<chem>C[C@H](CCCC(C)C)[C@H]1CC[C@@H]2[C@@]1(CC[C@H]3[C@H]2CC=C4[C@@]3(CC(C4)OC(=O)Cc5ccc(cc5)N(CCC)CCCl)C)C</chem>
InChI	SPJCRMJCFSJKDE-Z WBUGVOYSA-N
InChIKey	1S/C39H59Cl2NO2/c1-27(2)7-6-8-28(3)34-15-16-35-33-14-11-30-19-38(30,4)36(33)18-20-39(34,35)5)44-37(43)25-29-9-12-31(13-11)21-40)24-22-41/h9-13,27-28,32-36H,6-8,14-26H2,1-5H3/t28-,32+,33+,34-,35+,36+,38+,39-/m1/s1
log P (octanol-water)	13.12
Atmospheric OH Rate Constant	2.82E-10 cm ³ /molecule-sec
Melting Point	90 ° C



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