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## Typical Product Specifications & Properties

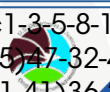
# BENZOIC ACID, 4-(TRANS-4-PENTYLCYCLOHEXYL)-, (1R)-1-PHENYL-1,2-ETHANEDIYL ESTER

CAS Number : 154102-21-3

Specifications	Limits
Canonicalized Compound	1
Compound Complexity	893
Hydrogen Bond Acceptor Count	4
Rotatable Bond Count	18
Allowed IUPAC Name	[(2R)-2-[4-(4-pentylcyclohexyl)benzoyl]oxy-2-phenyl-ethyl] 4-(4-pentylcyclohexyl)benzoate
CAS-like Style IUPAC Name	4-(4-pentylcyclohexyl)benzoic acid [(2R)-2-[oxo-[4-(4-pentylcyclohexyl)phenyl]methoxy]-2-phenylethyl] ester
Markup IUPAC Name	[(2<I>R</I>)-2-[4-(4-pentylcyclohexyl)benzoyl]oxy-2-phenylethyl] 4-(4-pentylcyclohexyl)benzoate
Preferred IUPAC Name	[(2R)-2-[4-(4-pentylcyclohexyl)benzoyl]oxy-2-phenylethyl] 4-(4-pentylcyclohexyl)benzoate
Systematic IUPAC Name	[(2R)-2-[4-(4-pentylcyclohexyl)phenyl]carbonyloxy-2-phenyl-ethyl] 4-(4-pentylcyclohexyl)benzoate
Traditional IUPAC Name	4-(4-amylcyclohexyl)benzoic acid [(2R)-2-[4-(4-amylcyclohexyl)benzoyl]oxy-2-phenyl-ethyl] ester
Standard InChI	InChI=1S/C44H58O4/c1-3-5-8-12-33-16-20-35(21-17-33)37-24-28-40(29-25-37)43(45)47-32-42(39-41)10-7-11-15-39)46-44(46)41-30-26-38(27-31-41)36-22-18-34(19-23-36)13-9-6-4-2/h7,10-11,14-15,24-31,33-36,42H,3-6,8-9,12-13,16-23,32H2,1-2H3/t33?,34?,35?,36?,42-/m0/s1



Standard InChI



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Standard  
InChIKey

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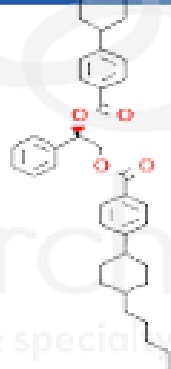
Specifications	Limits
XLogP3-AA Log P	14.8
Exact Mass	650.43351033
Molecular Weight	650.9
Canonical SMILES	<chem>CCCCC1CCC(CC1)C2=CC=C(C=C2)C(=O)OCC(C3=CC=C(C=C3)OC(=O)C4=CC=C(C=C4)C5CCC(CC5)CCC</chem>
Isomeric SMILES	<chem>CCCCC1CCC(CC1)C2=CC=C(C=C2)C(=O)OC[C@H](C3=CC=CC=C3)OC(=O)C4=CC=C(C=C4)C5CCC(CC5)CCC</chem>
Polar Surface Area	52.6
Topological	
Specifications	Limits
Monoisotopic Weight	650.43351033

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