Typical Product Specifications & Properties

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

CAS Number: : 154102-21-3

Specifications	Limits
Chemical Structure	615604 615604_benzoic-acid-4-trans-4-pentylcyclohexyl-1r-1-phenyl-1-2-ethanediyl-ester.png chemical structure
Molecular Formula	C44H58O4
Molecular weight	
Canonicalized Compound	1
Compound Complexity	893
Hydrogen Bond Acceptor Count	4
Hydrogen Bond Donor Count	
Rotatable Bond Count	18
Chemical Structure	chemicalStructure-benzoic-acid-4-trans-4-pentylcyclohexyl--1r-1-phenyl-1-2-ethanediyl-ester
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

Specifications	Limits
Preferred IUPAC Name	[(2R)-2-[4-(4-pentylcyclohexyl)benzoyl]oxy-2-phenylethyl] 4-(4-p
Systematic IUPAC Name	[(2R)-2-[4-(4-pentylcyclohexyl)phenyl]carbonyloxy-2-phenyl-eth
Traditional IUPAC Name	4-(4-amylcyclohexyl)benzoic acid [(2R)-2-[4-(4-amylcyclohexy
Standard InChI	InChI=1S/C44H58O4/c1-3-5-8-12-33-16-20-35(21-17-33)37-24-28-44(46)41-30-26-38(27-31-41)36-22-18-34(19-23-36)13-9-6-4-2/h7,2H3/t33?,34?,35?,36?,42-/m0/s1
Standard InChIKey	KTIVHFRVDVVCHK-BAFIUCHISA-N
XLogP3-AA Log P	14.8
Exact Mass	650.43351033

Specifications	Limits
Molecular Weight	650.9
Canonical SMILES	CCCCCC1CCC(CC1)C2=CC=C(C=C2)C(=O)OCC(C3=CC=C
Isomeric SMILES	CCCCCC1CCC(CC1)C2=CC=C(C=C2)C(=O)OC[C@@H]

SMILES	(C3=CC=CC=C3)OC(=O)C4=CC=C(C=C4)C5CCC(CC5)CCC
Polar Surface Area Topological	52.6
Monolsotopic Weight	650.43351033

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