Typical Product Specifications & Properties

Benzeneacetic acid, a-methyl-4-(2-methylpropyl)-, methyl ester, (aS)-

CAS Number: : 81576-55-8

Specifications	Limits
Molecular Formula	C14H20O2
Molecular weight	
Canonicalized Compound	1
Compound Complexity	215
Hydrogen Bond Acceptor Count	2
Hydrogen Bond Donor Count	
Rotatable Bond Count	5
Allowed IUPAC Name	methyl (2S)-2-(4-isobutylphenyl)propanoate
CAS-like Style IUPAC Name	(2S)-2-[4-(2-methylpropyl)phenyl]propanoic acid methyl ester
Markup IUPAC Name	methyl (2<I>S</I>)-2-[4-(2-methylpropyl)phenyl]propanoate
Preferred IUPAC Name	methyl (2S)-2-[4-(2-methylpropyl)phenyl]propanoate
Systematic IUPAC Name	methyl (2S)-2-[4-(2-methylpropyl)phenyl]propanoate

Specifications	Limits
Traditional IUPAC Name	(2S)-2-(4-isobutylphenyl)propionic acid methyl ester
Standard InChI	InChI=1S/C14H20O2/c1-10(2)9-12-5-7-13(8-6-12)11(3)14(15)16-4/h5-8,10-11H,9H2,1-4H3/t11-/m0/s1
Standard InChIKey	YNZYUHPFNYBBFF-NSHDSACASA-N
Exact Mass	220.146329876
Molecular Weight	220.31
Canonical SMILES	CC(C)CC1=CC=C(C=C1)C(C)C(=O)OC
Isomeric SMILES	C[C@@H](C1=CC=C(C=C1)CC(C)C)C(=O)OC
Polar Surface Area Topological	26.3
Monolsotopic Weight	220.146329876
XLogP3 Log P	3.8
Chemical Structure	chemicalStructure-benzeneacetic-acid-a-methyl-4-2-methylpropyl-methyl-ester-as-