Typical Product Specifications & Properties

Dibenzoyl-L-tartaric acid

CAS Number: : 2743-38-6

Specifications	Limits
Molecular Formula	C18H14O8
Molecular weight	
Canonicalized Compound	1
Compound Complexity	483
Hydrogen Bond Acceptor Count	8
Hydrogen Bond Donor Count	2
Traditional IUPAC Name	(2R,3R)-2,3-dibenzoyloxysuccinic acid
Rotatable Bond Count	9
Allowed IUPAC Name	(2R,3R)-2,3-dibenzoyloxybutanedioic acid
CAS-like Style IUPAC Name	(2R,3R)-2,3-dibenzoyloxybutanedioic acid
Markup IUPAC Name	(2<I>R</I>,3<I>R</I>)-2,3-dibenzoyloxybutanedioic acid
Preferred IUPAC Name	(2R,3R)-2,3-dibenzoyloxybutanedioic acid

Specifications	Limits
Systematic IUPAC Name	(2R,3R)-2,3-bis(phenylcarbonyloxy)butanedioic acid
Standard InChI	InChI=1S/C18H14O8/c19-15(20)13(25-17(23)11-7-3-1-4-8-11)14(16(21)22)26-18(24)12-9-5-2-6-10-12/h1-10,13-14H,(H,19,20)(H,21,22)/t13-,14-/m1/s1
Standard InChIKey	YONLFQNRGZXBBF-ZIAGYGMSSA-N
XLogP3-AA Log P	2.6
Exact Mass	358.06886740
Molecular Weight	358.3
Canonical SMILES	C1=CC=C(C=C1)C(=O)OC(C(C(=O)O)OC(=O)C2=CC=CC=C
Isomeric SMILES	C1=CC=C(C=C1)C(=O)O[C@H]([C@H](C(=O)O)OC(=O)C2=CC=CC=C2)C(=O)O
Polar Surface Area Topological	127
MonoIsotopic Weight	358.06886740
Chemical Structure	chemicalStructure-dibenzoyl-l-tartaric-acid