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Typical Product Specifications & Properties

2-Phenethyl hexanoate

CAS Number : 6290-37-5

Specifications	Limits
Chemical Structure	 chemicalStructure-2-phenethyl-hexanoate
Molecular Formula	C14H20O2
Molecular weight	
Canonicalized Compound	1
Compound Complexity	183
Hydrogen Bond Acceptor Count	2
Hydrogen Bond Donor Count	
Rotatable Bond Count	8
Allowed IUPAC Name	2-phenylethyl hexanoate
CAS-like Style IUPAC Name	hexanoic acid 2-phenylethyl ester
Markup IUPAC Name	2-phenylethyl hexanoate
Preferred IUPAC Name	2-phenylethyl hexanoate



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Specifications	Limits
Systematic IUPAC Name	2-phenylethyl hexanoate
Traditional IUPAC Name	hexanoic acid phenethyl ester
Standard InChI	InChI=1S/C14H20O2/c1-2-3-5-10-14(15)16-12-11-13-8-6-4-7-9-13/h4,6-9H,2-3,5,10-12H2,1H3
Standard InChIKey	BUYNWUMUDHPPDS-UHFFFAOYSA-N
Exact Mass	220.146329876
Molecular Weight	220.31
Canonical SMILES	<chem>CCCCC(=O)OCCc1ccccc1</chem>
Isomeric SMILES	<chem>CCCCC(=O)OCCc1ccccc1</chem>
Polar Surface Area Topological	26.3
Monoisotopic Weight	220.146329876
XLogP3 Log P	4.2



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