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Typical Product Specifications & Properties

Cyclohexanone, 4-propoxy-

CAS Number: : 158836-67-0

Specifications	Limits
Rotatable Bond Count	3
Allowed IUPAC Name	4-propoxycyclohexanone
CAS-like Style IUPAC Name	4-propoxy-1-cyclohexanone
Markup IUPAC Name	4-propoxycyclohexan-1-one
Preferred IUPAC Name	4-propoxycyclohexan-1-one
Systematic IUPAC Name	4-propoxycyclohexan-1-one
Molecular Formula	C ₉ H ₁₆ O ₂
Molecular weight	
Canonicalized Compound	1
Compound Complexity	122
Hydrogen Bond Acceptor Count	2
Hydrogen Bond Donor Count	



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Specifications	Limits
Traditional IUPAC Name	4-propoxycyclohexanone
Standard InChI	InChI=1S/C9H16O2/c1-2-7-11-9-5-3-8(10)4-6-9/h9H,2-7H2,1H3
Standard InChIKey	XHLFNDRDYLLAEV-UHFFFAOYSA-N
XLogP3-AA Log P	1.2
Exact Mass	156.115029749
Molecular Weight	156.22
Canonical SMILES	CCCOC1CCC(=O)CC1
Isomeric SMILES	CCCOC1CCC(=O)CC1
Polar Surface Area Topological	26.3
Chemical Structure	 615596 615596_cyclohexanone-4-propoxy-.png chemical structure
Monoisotopic Weight	156.115029749
Chemical Structure	 chemicalStructure-cyclohexanone-4-propoxy-



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