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Typical Product Specifications & Properties

1,4-Diphenyl-1-butanone

CAS Number: : 5407-91-0

Specifications	Limits
Molecular weight	224.30
EINECS	226-471-4
SMILES	<chem>c1ccc(C(=O)CCCC2CCCCC2)cc1</chem>
InChI	1S/C16H16O/c17-16(15-11-5-2-6-12-15)13-7-10-14-8-3-1-4-9-14/h1-6,8-9,11-12H,7,10,13H2
InChIKey	GBUMEGLMTNAXOM-UHFFFAOYSA-N
Molecular weight	303.83
EINECS	219-567-2
SMILES	<chem>C(c1ccc(N(C)C)cc1)(c1ccc(N(C)C)cc1)=N.Cl</chem>
InChI	1S/C17H21N3.ClH/c1-19(2)15-9-5-13(6-10-15)17(18)14-7-11-16(12-8-14)20(3)4;/h5-12,18H,1-4H3;1H
InChIKey	KSCQDDRPFHTIRL-UHFFFAOYSA-N
Water solubility	Soluble in water or ethanol
Stability	Stable. Incompatible with strong oxidizing agents.



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Specifications	Limits
Colour Index	41000
Storage Temperature	Store at room temperature.
Melting Point	>250 °C (dec.)
Atmospheric OH Rate Constant	2.05E-10 cm ³ /molecule-sec
log P (octanol-water)	2.980
Water solubility	1.00E+04 mg/L
Henry's Law Constant	3.64E-09 atm-m ³ /mole
Vapor Pressure	1.29E-06 mm Hg



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