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Typical Product Specifications & Properties

3-Heptanone, 6-(dimethylamino)-4,4-diphenyl-

CAS Number: : 76-99-3

Specifications	Limits
Molecular weight	309.45
EINECS	200-996-9
SMILES	<chem>CCC(=O)C(CC(C)N(C)C)(c1ccccc1)c2ccccc2</chem>
InChI	1S/C21H27NO/c1-5-20(23)21(16-17(2)22(3)4,18-12-8-6-9-13-18)19-14-10-7-11-15-19/h6-15,17H,5,16H2,1-4H3
InChIKey	USSIQXCVUWKGNF-UHFFFAOYSA-N
Atmospheric OH Rate Constant	1.05E-10 cm ³ /molecule-sec
Henry's Law Constant	4.97E-10 atm-m ³ /mole
log P (octanol-water)	3.93
Water solubility	48.5 mg/L
Vapor Pressure	1.12E-06 mm Hg
pKa Dissociation Constant	8.94



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415 Huguenot Street, New Rochelle, New York 10801

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