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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 <sup>3</sup> /molecule-sec  |
| Henry's Law Constant         | 4.97E-10 atm-m <sup>3</sup> /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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