Pyrovalerone

Other names: 4'-Methyl-2-(1-pyrrolidinyl)valerophenone
Inchi: InChI=1S/C16H23NO/c1-3-6-15(17-11-4-5-12-17)16(18)14-9-7-13(2)8-10-14/h7-10,15H,
InchiKey: SWUVZKWCOBGPTH-UHFFFAOYSA-N
Formula: C16H23NO
SMILES: CCCC(C(=O)c1ccc(C)cc1)N1CCCC1
Mol. weight [g/mol]: 245.36
CAS: 3563-49-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Crippen Method
logp	3.442		Crippen Method
mcvol	213.230	ml/mol	McGowan Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3563493&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume