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

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