4-Methyl-a-pyrrolidinobutiophenone

Other names: 4 -methyl-«alpha»-pyrrolidinobutyrophenone
Inchi: InChI=1S/C15H21NO/c1-3-14(16-10-4-5-11-16)15(17)13-8-6-12(2)7-9-13/h6-9,14H,3-5,1
InchiKey: NXNPGAAZKYDOPW-UHFFFAOYSA-N
Formula: C15H21NO
SMILES: CCC(C(=O)c1ccc(C)cc1)N1CCCC1
Mol. weight [g/mol]: 231.33
CAS: 1214-15-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.70		Crippen Method
logp	3.052		Crippen Method
mcvol	199.140	ml/mol	McGowan Method
rinpol	1790.00		NIST Webbook
rinpol	1790.00		NIST Webbook

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=C1214159&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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