4'-Methyl-a-pyrrolidinopropiophenone

Other names: Pyrrolidine, 1-(1-(4-methylbenzoyl)ethyl)
Inchi: InChI=1S/C14H19NO/c1-11-5-7-13(8-6-11)14(16)12(2)15-9-3-4-10-15/h5-8,12H,3-4,9-10
InchiKey: APSJUNFBAXIXLK-UHFFFAOYSA-N
Formula: C14H19NO
SMILES: Cc1ccc(C(=O)C(C)N2CCCC2)cc1
Mol. weight [g/mol]: 217.31
CAS: 1313393-58-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.28		Crippen Method
logp	2.662		Crippen Method
mcvol	185.050	ml/mol	McGowan Method
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1725.00		NIST Webbook

Sources

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=C1313393586&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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