a-Pyrrolidinopropiophenone

Other names: Pyrrolidine, 1-(1-benzoylethyl)
Inchi: InChI=1S/C13H17NO/c1-11(14-9-5-6-10-14)13(15)12-7-3-2-4-8-12/h2-4,7-8,11H,5-6,9-1
InchiKey: KPUJAQRFIJAORQ-UHFFFAOYSA-N
Formula: C13H17NO
SMILES: CC(C(=O)c1ccccc1)N1CCCC1
Mol. weight [g/mol]: 203.28
CAS: 92040-10-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.80		Crippen Method
logp	2.354		Crippen Method
mcvol	170.960	ml/mol	McGowan Method
rinpol	1595.00		NIST Webbook
rinpol	1595.00		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=C92040103&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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