

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,3-4,9-10H
InchiKey:	APSJUNFBAXIXLK-UHFFFAOYSA-N
Formula:	C14H19NO
SMILES:	<chem>Cc1ccc(C(=O)C(C)N2CCCC2)cc1</chem>
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
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rinpol	1725.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1313393586&Units=SI
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

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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