

4-Piperidinone, 3-methyl-1-(phenylmethyl)-

Other names:	4-Piperidone, 1-benzyl-3-methyl- 1-Benzyl-3-methyl-4-piperidone N-Benzyl-3-methyl-4-piperidone 1-Benzyl-3-methyl-piperidin-4-one
Inchi:	InChI=1S/C13H17NO/c1-11-9-14(8-7-13(11)15)10-12-5-3-2-4-6-12/h2-6,11H,7-10H2,1H3
InchiKey:	OVQAJYCAXPHYNV-UHFFFAOYSA-N
Formula:	C13H17NO
SMILES:	CC1CN(Cc2ccccc2)CCC1=O
Mol. weight [g/mol]:	203.28
CAS:	34737-89-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	2.098		Crippen Method
mcvol	170.960	ml/mol	McGowan Method
rinpol	1719.00		NIST Webbook
rinpol	1719.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C34737898&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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