

4-phenyl-4-piperidinocyclohexanol

Inchi: InChI=1S/C17H25NO/c19-16-9-11-17(12-10-16,15-7-3-1-4-8-15)18-13-5-2-6-14-18/h1,3-17
InchiKey: KPRUAZBLIREHPD-UHFFFAOYSA-N
Formula: C17H25NO
SMILES: OC1CCC(c2ccccc2)(N2CCCCC2)CC1
Mol. weight [g/mol]: 259.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	3.303		Crippen Method
mcvol	220.760	ml/mol	McGowan Method
rinpol	2549.00		NIST Webbook
rinpol	2549.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R139570&Units=SI>
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>

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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<https://www.chemeo.com/cid/90-460-1/4-phenyl-4-piperidinocyclohexanol.pdf>

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