3-phenyl-3-piperidinocyclohexanol (TMS)

Inchi: InChI=1S/C17H25NO/c19-16-10-7-11-17(14-16,15-8-3-1-4-9-15)18-12-5-2-6-13-18/h1,3-
InchiKey: NHEKQIGDKRYTQF-UHFFFAOYSA-N
Formula: C17H25NO
SMILES: OC1CCCC(c2ccccc2)(N2CCCCC2)C1
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	2343.00		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=R139565&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

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