4-phenyl-4-piperidinocyclohexanol (TMS)

Inchi: InChI=1S/C20H33NOSi/c1-23(2,3)22-19-12-14-20(15-13-19,18-10-6-4-7-11-18)21-16-8-5

InchiKey: GLJNUJZJDUXBDT-UHFFFAOYSA-N

Formula: C20H33NOSi

SMILES: C[Si](C)(C)OC1CCC(c2ccccc2)(N2CCCCC2)CC1

Mol. weight [g/mol]: 331.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	5.162		Crippen Method
rinpol	2372.00		NIST Webbook
rinpol	2372.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R139585&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices