

1-(1-phenylcyclohexyl)-4-hydroxypiperidine (TMS)

Inchi: InChI=1S/C20H33NOSi/c1-23(2,3)22-19-12-16-21(17-13-19)20(14-8-5-9-15-20)18-10-6-4
InchiKey: JCWNOHZBVWIOGH-UHFFFAOYSA-N
Formula: C20H33NOSi
SMILES: C[Si](C)(C)OC1CCN(C2(c3ccccc3)CCCC2)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	2380.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R139550&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/11-821-7/1-1-phenylcyclohexyl-4-hydroxypiperidine-TMS.pdf>

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