1-(1-phenyl-4-hydroxycyclohexyl)-4-hydroxypiper (TMS)

InChI: InChI=1S/C23H41NO2Si2/c1-27(2,3)25-21-12-16-23(17-13-21,20-10-8-7-9-11-20)24-18-

InChIKey: XBODLZZCEUQVJY-UHFFFAOYSA-N

Formula: C23H41NO2Si2

SMILES: C[Si](C)(C)OC1CCN(C2(c3ccccc3)CCC(O[Si](C)(C)C)CC2)CC1

Mol. weight [g/mol]: 419.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.58		Crippen Method
logp	5.992		Crippen Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R139510&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

rinpol: Non-polar retention indices

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