

Allo-pregnenediol, MO TMS

Inchi: InChI=1S/C27H52O2Si2/c1-19(28-30(4,5)6)23-12-13-24-22-11-10-20-18-21(29-31(7,8)9)
InchiKey: PSZRAFDARWUCMW-UDVYNZHDSA-N
Formula: C27H52O2Si2
SMILES: CC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 464.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.51		Crippen Method
logp	8.105		Crippen Method
rinpol	2762.00		NIST Webbook
rinpol	2791.00		NIST Webbook
rinpol	2803.00		NIST Webbook
rinpol	2785.00		NIST Webbook
rinpol	2762.00		NIST Webbook
rinpol	2785.00		NIST Webbook
rinpol	2776.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R149458&Units=SI>

Legend

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

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