

Allopregnanediol TMS

Inchi: InChI=1S/C28H54O2Si2/c1-10-26(30-32(7,8)9)25-14-13-23-22-12-11-20-19-21(29-31(4,5)6)33-27-24-28-34-35-36-37-38-39-40-41-42-43-44-45-46-47-48-49-50-51-52-53-54-55-56-57-58-59-60-61-62-63-64-65-66-67-68-69-70-71-72-73-74-75-76-77-78-79-80-81-82-83-84-85-86-87-88-89-90-91-92-93-94-95-96-97-98-99-100
InchiKey: FFOITQMJIMFGSD-BBEQGNITSA-N
Formula: C28H54O2Si2
SMILES: CCC(O[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 478.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	8.495		Crippen Method
rinpol	2783.00		NIST Webbook
rinpol	2796.00		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=R97620&Units=SI>

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.chemeo.com/cid/53-561-0/Allopregnanediol-TMS.pdf>

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