

Desoxycohumulone, TMS

Inchi: InChI=1S/C29H52O4Si3/c1-20(2)16-18-23-27(31-34(7,8)9)24(19-17-21(3)4)29(33-36(13)
InchiKey: YREKGLSESCDUID-UHFFFAOYSA-N
Formula: C29H52O4Si3
SMILES: CC(C)=CCc1c(O[Si](C)(C)C)c(CC=C(C)C)c(O[Si](C)(C)C)c(C(=O)C(C)C)c1O[Si](C)(C)C
Mol. weight [g/mol]: 548.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.58		Crippen Method
logp	9.184		Crippen Method
rinpol	2299.00		NIST Webbook
rinpol	2299.00		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=R97040&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/33-331-7/Desoxycohumulone-TMS.pdf>

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