

Desoxyhumulone, TMS

Inchi: InChI=1S/C30H54O4Si3/c1-21(2)16-18-24-28(32-35(7,8)9)25(19-17-22(3)4)30(34-37(13)
InchiKey: RKJDXNQMWHFDSX-UHFFFAOYSA-N
Formula: C30H54O4Si3
SMILES: CC(C)=CCc1c(O[Si](C)(C)C)c(CC=C(C)C)c(O[Si](C)(C)C)c(C(=O)CC(C)C)c1O[Si](C)(C)
Mol. weight [g/mol]: 563.00

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.99		Crippen Method
logp	9.574		Crippen Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R97068&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/12-439-1/Desoxyhumulone-TMS.pdf>

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