

trans-Dehydrohumulinic acid, TMS

Inchi: InChI=1S/C21H36O4Si2/c1-14(2)11-12-16-19(23)21(25-27(8,9)10)18(17(22)13-15(3)4)2
InchiKey: YIORPTTUNYARET-UHFFFAOYSA-N
Formula: C₂₁H₃₆O₄Si₂
SMILES: CC(C)=CCC1=C(O[Si](C)(C)C)C(C(=O)CC(C)C)=C(O[Si](C)(C)C)C1=O
Mol. weight [g/mol]: 408.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.65		Crippen Method
logp	5.752		Crippen Method
rinpol	2293.00		NIST Webbook
rinpol	2330.00		NIST Webbook
rinpol	2293.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R384200&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/114-941-0/trans-Dehydrohumulinic-acid-TMS.pdf>

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