

epi-Me-dihydrophaseic acid-TMS

Inchi: InChI=1S/C21H38O5Si2/c1-16(12-18(22)23)10-11-21(26-28(7,8)9)19(2)13-17(25-27(4,5)
InchiKey: FYXIGEQQZCDOMY-SSVOVMCRSA-N
Formula: C21H38O5Si2
SMILES: CC(C=CC1(O[Si](C)(C)C)C2(C)COC1(C)CC(O[Si](C)(C)C)C2)=CC(=O)O
Mol. weight [g/mol]: 426.69

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.67		Crippen Method
logp	4.973		Crippen Method
rinpol	2177.00		NIST Webbook
rinpol	2177.00		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=R487453&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/31-575-9/epi-Me-dihydrophaseic-acid-TMS.pdf>

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