

ent-6«alpha»,7«alpha»-Dihydroxytrachylobanic acid, Me-TMS

Inchi: InChI=1S/C27H48O4Si2/c1-24-12-11-13-25(2,23(28)29-4)21(24)20(30-32(5,6)7)22(31-3)
InchiKey: RNTLIJIWMLSSHA-UZIUJYAZSA-N
Formula: C27H48O4Si2
SMILES: COC(=O)C1(C)CCCC2(C)C1C(O[Si](C)(C)C)C(O[Si](C)(C)C)C13CC4C(CC21)C4(C)C3
Mol. weight [g/mol]: 492.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.03		Crippen Method
logp	6.478		Crippen Method
rinpol	2531.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R559112&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/49-144-8/ent-6-alpha-7-alpha-Dihydroxy-trachylobanic-acid-Me-TMS.pdf>

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