

17-epi-Bolasterone, per-TMS

Inchi: InChI=1S/C27H48O2Si2/c1-19-17-20-18-21(28-30(5,6)7)11-14-25(20,2)22-12-15-26(3)2
InchiKey: FKNAXZNQYPTDCN-FIHZUOIASA-N
Formula: C27H48O2Si2
SMILES: CC1C=C2C=C(O[Si](C)(C)C)CCC2(C)C2CCC3(C)C(CCC3(C)O[Si](C)(C)C)C12
Mol. weight [g/mol]: 460.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.84		Crippen Method
logp	8.151		Crippen Method
rinpol	2728.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R257702&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/46-863-3/17-epi-Bolasterone-per-TMS.pdf>

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