

Epiaethiocholanolone, MO-TBDMS

Inchi: InChI=1S/C26H47NO2Si/c1-24(2,3)30(7,8)29-19-13-15-25(4)18(17-19)9-10-20-21-11-12
InchiKey: ATAVHXFPXLCEHX-OXNAYYIJSA-N
Formula: C26H47NO2Si
SMILES: CON=C1CCC2C3CCC4CC(O[Si](C)(C)C(C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 433.74

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.33		Crippen Method
logp	7.422		Crippen Method
rinpol	2830.00		NIST Webbook
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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=R594393&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/115-248-9/Epiaethiocholanolone-MO-TBDMS.pdf>

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