

3«beta»-Trimethylsilyloxy-30-norlupan-20-one

Inchi: InChI=1S/C32H56O2Si/c1-21(33)22-13-16-29(4)19-20-31(6)23(27(22)29)11-12-25-30(5)
InchiKey: CWQUWBSFGPDZNL-PFPGRZSESA-N
Formula: C32H56O2Si
SMILES: CC(=O)C1CCC2(C)CCC3(C)C(CCC4C5(C)CCC(O[Si](C)(C)C)C(C)(C)C5CCC43C)C12
Mol. weight [g/mol]: 500.87

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.80		Crippen Method
logp	8.897		Crippen Method
rinpol	3460.00		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=R583447&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/49-167-3/3-beta-Trimethylsilyloxy-30-norlupan-20-one.pdf>

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