

(20R)-3«beta»-Acetoxy-29-(trimethylsilyloxy)lupane

Inchi: InChI=1S/C35H62O3Si/c1-23(22-37-39(9,10)11)25-14-17-32(5)20-21-34(7)26(30(25)32)
InchiKey: CCMGLYUPVIXBBE-KMZXCFFSA-N
Formula: C35H62O3Si
SMILES: CC(=O)OC1CCC2(C)C(CCC3(C)C2CCC2C4C(C(C)CO[Si](C)(C)C)CCC4(C)CCC23C)C
Mol. weight [g/mol]: 558.95

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.40		Crippen Method
logp	9.507		Crippen Method
rinpol	3600.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R583303&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/55-804-8/20R-3-beta-Acetoxy-29-trimethylsilyloxy-lupane.pdf>

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