(20RS)-3«beta»-(Trimethylsilyloxy)lupan-29-al

Inchi: InChI=1S/C33H58O2Si/c1-22(21-34)23-13-16-30(4)19-20-32(6)24(28(23)30)11-12-26-31
InchiKey: WXWCILSVRGNVLM-NICBXEFUSA-N
Formula: C33H58O2Si
SMILES: CC(C=O)C1CCC2(C)CCC3(C)C(CCC4C5(C)CCC(O[Si](C)(C)C)C(C)(C)C5CCC43C)C12
Mol. weight [g/mol]: 514.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.98		Crippen Method
logp	9.143		Crippen Method
rinpol	3580.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R583323&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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