

3«beta»-(Trimethylsilyloxy)lup-20(29)-en-30-al

Inchi: InChI=1S/C33H56O2Si/c1-22(21-34)23-13-16-30(4)19-20-32(6)24(28(23)30)11-12-26-31
InchiKey: OWROAOZEHRQSAS-RTIKZPSZSA-N
Formula: C33H56O2Si
SMILES: C=C(C=O)C1CCC2(C)CCC3(C)C(CCC4C5(C)CCC(O[Si](C)(C)C)C(C)(C)C5CCC43C)C1
Mol. weight [g/mol]: 512.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.08		Crippen Method
logp	9.063		Crippen Method
rinpol	3510.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R583452&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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