

Ursolic aldehyde TMS ether

Inchi: InChI=1S/C33H56O2Si/c1-22-13-18-33(21-34)20-19-31(6)24(28(33)23(22)2)11-12-26-30
InchiKey: DPRCZECAUZRWCQ-UHFFFAOYSA-N
Formula: C33H56O2Si
SMILES: CC1CCC2(C=O)CCC3(C)C(=CCC4C5(C)CCC(O[Si](C)(C)C)C(C)(C)C5CCC43C)C2C1C
Mol. weight [g/mol]: 512.88

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.08		Crippen Method
logp	9.063		Crippen Method
rinpol	3668.60		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=U414387&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/98-989-7/Ursolic-aldehyde-TMS-ether.pdf>

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