

22-Ketocholesterol, TMS

Inchi: InChI=1S/C30H54O2Si/c1-20(2)9-14-28(31)21(3)25-12-13-26-24-11-10-22-19-23(32-33)
InchiKey: IAPAOYQMECJWJT-DARJXMCLSA-N
Formula: C30H54O2Si
SMILES: CC(C)CCC(=O)C(C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 474.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.31		Crippen Method
logp	8.507		Crippen Method
rinpol	3290.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R528688&Units=SI>

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/15-519-9/22-Ketocholesterol-TMS.pdf>

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