

23,24-Dinor-5-cholen-3-on-22-ol, TMS

Inchi: InChI=1S/C28H48O2Si/c1-18(2)26(30-31(6,7)8)19(3)23-11-12-24-22-10-9-20-17-21(29)1
InchiKey: PVSQWUJLSKZFOD-LXIGCDK TSA-N
Formula: C28H48O2Si
SMILES: CC(C)C(O[Si](C)(C)C)C(C)C1CCC2C3CC=C4CC(=O)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 444.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.57		Crippen Method
logp	7.647		Crippen Method
rinpol	3030.00		NIST Webbook
rinpol	3030.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R11705&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/27-903-9/23-24-Dinor-5-cholen-3-on-22-ol-TMS.pdf>

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