

5-Cholen-3-on-24-ol, TMS

Inchi: InChI=1S/C30H52O2Si/c1-20(2)28(32-33(6,7)8)14-9-21(3)25-12-13-26-24-11-10-22-19-2
InchiKey: XISQWTADYGZVLW-GXWLHDSLSA-N
Formula: C30H52O2Si
SMILES: CC(C)C(CCC(C)C1CCC2C3CC=C4CC(=O)CCC4(C)C3CCC12C)O[Si](C)(C)C
Mol. weight [g/mol]: 472.82

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.41		Crippen Method
logp	8.427		Crippen Method
rinpol	3275.00		NIST Webbook
rinpol	3275.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R11844&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/37-091-0/5-Cholen-3-on-24-ol-TMS.pdf>

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