

24-Nor-5B-Cholan-3A,7A,12A,23-tetrol, TMS

Inchi: InChI=1S/C35H72O4Si4/c1-25(19-21-36-40(4,5)6)28-16-17-29-33-30(24-32(35(28,29)3))
InchiKey: AZJYCBBVNRRNOD-YYRNYOZSA-N
Formula: C35H72O4Si4
SMILES: CC(CCO[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C1C
Mol. weight [g/mol]: 669.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.01		Crippen Method
logp	10.403		Crippen Method
rinpol	3166.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R585067&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/49-099-9/24-Nor-5B-Cholan-3A-7A-12A-23-tetrol-TMS.pdf>

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