

5B-Cholestane-3A,7A,12A,24R,25-pentol, TMS

Inchi: InChI=1S/C42H88O5Si5/c1-30(21-24-37(45-50(12,13)14)40(2,3)47-52(18,19)20)33-22-2
InchiKey: QOKBFGNTFZLJGF-GNYWDRPSSA-N
Formula: C42H88O5Si5
SMILES: CC(CCC(O[Si](C)(C)C)C(C)(C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)C5
Mol. weight [g/mol]: 813.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.30		Crippen Method
logp	12.792		Crippen Method
rinpol	3619.00		NIST Webbook
rinpol	3619.00		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=R585121&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/123-884-4/5B-Cholestane-3A-7A-12A-24R-25-pentol-TMS.pdf>

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