

5B-Cholestane-3A,7A,12A,26-tetrol, TMS

Inchi: InChI=1S/C39H80O4Si4/c1-28(27-40-44(5,6)7)18-17-19-29(2)32-20-21-33-37-34(26-36)
InchiKey: FQRGIGVECJSGDA-WJMDMBSHSA-N
Formula: C39H80O4Si4
SMILES: CC(CCCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CC(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 725.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	11.819		Crippen Method
rinpol	3496.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R585156&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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