

5B-Cholestane-3A,7A,12A,25-tetrol, TMS

Inchi: InChI=1S/C39H80O4Si4/c1-28(19-18-23-37(2,3)43-47(15,16)17)31-20-21-32-36-33(27-3
InchiKey: ZRNUNTAJDOGHFB-FANUSJFJSA-N
Formula: C39H80O4Si4
SMILES: CC(CCCC(C)(C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C
Mol. weight [g/mol]: 725.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	11.962		Crippen Method
rinpol	3451.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R585141&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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