

5B-Cholestane-3A,7A,24S,25-tetrol, TMS

Inchi: InChI=1S/C39H80O4Si4/c1-28(18-21-35(42-46(12,13)14)37(2,3)43-47(15,16)17)31-19-2
InchiKey: FRJMTVKGUJKZCF-FANUSJFJSA-N
Formula: C39H80O4Si4
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)C4C1
Mol. weight [g/mol]: 725.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Crippen Method
logp	11.962		Crippen Method
rinpol	3628.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R585181&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/49-020-5/5B-Cholestane-3A-7A-24S-25-tetrol-TMS.pdf>

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