

5B-Cholane-3A,7A,24-triol, TMS

Inchi: InChI=1S/C33H66O3Si3/c1-24(14-13-21-34-37(4,5)6)27-15-16-28-31-29(18-20-33(27,28)32)30-25-26-22-23-35-36-29
InchiKey: DIDRNKWXWKOIP-RHHLZHACSA-N
Formula: C33H66O3Si3
SMILES: CC(CCCO[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCO
Mol. weight [g/mol]: 595.13

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	9.963		Crippen Method
rinpol	3251.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R585116&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/15-531-5/5B-Cholane-3A-7A-24-triol-TMS.pdf>

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