

acid, DMESI
InChI=1S/C40H80O5Si4/c1-16-46(8,9)42-31-24-27-39(7)34-25-26-38(6)32(30(5)20-23-3
InChIKey: JQYSIUTVAXNGBU-XWEMHBRLSA-N

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Formula: C₄₀H₈₀O₅Si₄

SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)CC)CC4(O[Si](C)(C)CC)CC(O[Si](C)(C)CC)CC4C3C2C1

Mol. weight [g/mol]: 753.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.12		Crippen Method
logp	12.024		Crippen Method
rinpol	3610.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279826&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/58-231-1/3-alpha-5-beta-7-beta-trihydroxy-5-beta-cholan-24-oic-acid-DMESI.pdf>

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