

acid, DMESI
InChIKey: RIWORMFFYCJZMM-AYROHMKFSA-N

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Formula: C₃₆H₇₀O₄Si₃

SMILES: CC[Si](C)(C)OC(=O)CCC(C)C1CCC2C3CCC4CC(O[Si](C)(C)CC)CCC4(C)C3CC(O[Si](C)

Mol. weight [g/mol]: 651.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.95		Crippen Method
logp	10.660		Crippen Method
rinpol	3410.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R279722&Units=SI>

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/45-802-1/3-alpha-12-alpha-dihydroxy-5-beta-cholan-24-oic-acid-DMESI.pdf>

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