

nor-Ursodesoxycholic acid, methyl ester, TMS

Other names:	Norursodeoxycholic acid, trimethylsilyl ether-methyl ester
Inchi:	InChI=1S/C30H56O4Si2/c1-20(17-27(31)32-4)23-11-12-24-28-25(14-16-30(23,24)3)29(2
InchiKey:	HCYJJSCVAJQMOY-ZGEKCCMESA-N
Formula:	C30H56O4Si2
SMILES:	COC(=O)CC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]:	536.93

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	7.895		Crippen Method
rinpol	3183.00		NIST Webbook
rinpol	3120.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R182782&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/68-334-6/nor-Ursodesoxycholic-acid-methyl-ester-TMS.pdf>

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