

Ursodeoxycholic acid, trimethylsilyl ether-methyl ester

Other names:	3«alpha»,7«beta»-Dihydroxy-5«beta»-cholanoic acid, MeTMS Ursodesoxycholic acid, methyl ester, TMS 3«alpha»,7«beta»-Dihydroxy-5«beta»-cholanoic acid, methyl ester-trimethylsilyl ether
Inchi:	InChI=1S/C31H58O4Si2/c1-21(11-14-28(32)33-4)24-12-13-25-29-26(16-18-31(24,25)3)3
InchiKey:	FUVKOFYYHKWFJK-ZVNZYJRCSA-N
Formula:	C31H58O4Si2
SMILES:	COC(=O)CCC(C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3CCC12O
Mol. weight [g/mol]:	550.96
CAS:	63813-73-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.81		Crippen Method
logp	8.285		Crippen Method
rinpol	3306.00		NIST Webbook
rinpol	3279.00		NIST Webbook
rinpol	3268.00		NIST Webbook
rinpol	3252.00		NIST Webbook
rinpol	3250.00		NIST Webbook
rinpol	3249.00		NIST Webbook
rinpol	3268.00		NIST Webbook
ripol	3752.00		NIST Webbook
ripol	3752.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63813730&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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