

Ursodeoxycholic acid, bis(trimethylsilyl) ether, trimethylsilyl ester

Other names:	Ursodeoxycholic acid, 3tms derivative
Inchi:	InChI=1S/C33H64O4Si3/c1-23(13-16-30(34)37-40(10,11)12)26-14-15-27-31-28(18-20-32)33
InchiKey:	TUMUEXLHVCPQOP-UHFFFAOYSA-N
Formula:	C33H64O4Si3
SMILES:	CC(CCC(=O)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)CC4CC(O[Si](C)(C)C)CCC4(C)C3
Mol. weight [g/mol]:	609.12

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	9.490		Crippen Method
rmpol	3336.30		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352609&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
rmpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/118-792-2/Ursodeoxycholic-acid-bis-trimethylsilyl-ether-trimethylsilyl-ester.pdf>

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