Cholan-24-oic acid, 3,7-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester, (3«alpha»,5«beta»,7«alpha»)-

Othernames:	Trimethylsilyl 3,7-bis[(trimethylsilyl)oxy]cholan-24-oate, (3«alpha»,5«beta»,7«alpha»)-, Chenodeoxycholic acid, bis(trimethylsilyl) ether, trimethylsilyl ester
	Trimethylsilyl (3«alpha»,5«beta»,7«alpha»)-3,7-bis[(trimethylsilyl)oxy]cholan-24-oate
	3«alpha»,7«alpha»-dihydroxy-5«beta»-cholan-24-oic acid, tris-TMS
	3«alpha»,7«alpha»-dihydroxy-5«beta»-cholan-24-oic acid, TMS
	3«alpha»,7«beta»-dihydroxy-5«beta»-cholan-24-oic acid, TMS
	Chenodeoxycholic acid, (3«alpha»,5«beta»,7«alpha»)-, 3tms
Inchi:	InChI=1S/C33H64O4Si3/c1-23(13-16-30(34)37-40(10,11)12)26-14-15-27-31-28(18-20-33
InchiKey:	TUMUEXLHVCPQOP-XQNMAFGOSA-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
CAS:	55320-14-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.05		Cheméo Relay (1.0)
logp	9.490		Crippen Method
rinpol	3235.00		NIST Webbook
rinpol	3240.00		NIST Webbook
rinpol	3282.00		NIST Webbook
rinpol	3287.00		NIST Webbook
rinpol	3235.00		NIST Webbook
tf	383.27	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55320144&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
tf:	Normal melting (fusion) point