

5-Cholenoic acid, 3-«beta»-hydroxy, methyl ester, TMS

Other names:

3-«beta»-Hydroxy-5-cholenoic acid, MeTMS

Methyl 3-«beta»-hydroxy-5-cholenoate, TMS

3-«beta»-Hydroxy-5-cholenoic acid, methyl ester, TMS

Inchi:

InChI=1S/C28H48O3Si/c1-19(8-13-26(29)30-4)23-11-12-24-22-10-9-20-18-21(31-32(5,6)

InchiKey:

XCHAAEKPDWQLIP-LFKYXLBRSA-N

Formula:

C28H48O3Si

SMILES:

COC(=O)CCC(C)C1CCC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C

Mol. weight [g/mol]:

460.76

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	7.375		Crippen Method
rinpol	3192.00		NIST Webbook
rinpol	3192.00		NIST Webbook
rinpol	3175.00		NIST Webbook
rinpol	3174.00		NIST Webbook
rinpol	3172.00		NIST Webbook
rinpol	3174.00		NIST Webbook
rinpol	3192.00		NIST Webbook
rinpol	3175.00		NIST Webbook

Sources

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=R389998&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

log10ws:

Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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