

5-Cholesten-3-«beta»,7-«alpha»,25,26-tetrol, TMS

Inchi:	InChI=1S/C39H78O4Si4/c1-29(18-17-23-37(2,43-47(14,15)16)28-40-44(5,6)7)32-19-20-3
InchiKey:	LAWCYASJPRCMJQ-GXEDGXGOSA-N
Formula:	C39H78O4Si4
SMILES:	CC(CCCC(C)(CO[Si](C)(C)C)O[Si](C)(C)C)C1CCC2C3C(O[Si](C)(C)C)C=C4CC(O[Si](C)(C)C)C
Mol. weight [g/mol]:	723.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.78		Crippen Method
logp	11.884		Crippen Method
rinpol	3630.00		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=R390220&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

Latest version available from:

<https://www.chemeo.com/cid/51-610-7/5-Cholesten-3-beta-7-alpha-25-26-tetrol-TMS.pdf>

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