

ent-7«alpha»-Hydroxy trachylobanic acid, Me-TMS

Inchi:	InChI=1S/C24H40O3Si/c1-21-9-8-10-22(2,20(25)26-4)17(21)12-19(27-28(5,6)7)24-13-16
InchiKey:	NSQQWIMKIXFQDW-VBUXDKKWSA-N
Formula:	C24H40O3Si
SMILES:	COC(=O)C1(C)CCCC2(C)C1CC(O[Si](C)(C)C)C13CC4C(CC21)C4(C)C3
Mol. weight [g/mol]:	404.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	5.648		Crippen Method
rinpol	2399.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R559147&Units=SI

Legend

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

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