

1,4-Anhydromannitol, TMS

Inchi:	InChI=1S/C18H44O5Si4/c1-24(2,3)20-14-16(22-26(7,8)9)17-18(23-27(10,11)12)15(13-19)
InchiKey:	XFCGMMDSCXRHLA-BSDSXHPESA-N
Formula:	C18H44O5Si4
SMILES:	C[Si](C)(C)OCC(O[Si](C)(C)C)C1OCC(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]:	452.88

Physical Properties

Property code	Value	Unit	Source
log10ws	4.66		Crippen Method
logp	4.897		Crippen Method
rinpol	1878.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R74181&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
rinpol:	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/50-396-7/1-4-Anhydromannitol-TMS.pdf>

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