

1,5-Anhydromannitol, TMS

Inchi: InChI=1S/C18H44O5Si4/c1-24(2,3)20-14-15-17(22-26(7,8)9)18(23-27(10,11)12)16(13-19)
InchiKey: BKZSHWBRUJTUIK-XLAORIBOSA-N
Formula: C18H44O5Si4
SMILES: C[Si](C)(C)OCC1OCC(O[Si](C)(C)C)C(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	1804.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R74113&Units=SI>

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/66-756-0/1-5-Anhydromannitol-TMS.pdf>

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