

Sorbitol, 6-methyl, TMS

Inchi: InChI=1S/C22H56O6Si5/c1-23-17-19(25-30(5,6)7)21(27-32(11,12)13)22(28-33(14,15)16)
InchiKey: OAAGURLXCYYFBS-MLNNCEHLSA-N
Formula: C22H56O6Si5
SMILES: COCC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(CO[Si](C)(C)C)O[Si](C)(C)C
Mol. weight [g/mol]: 557.10

Physical Properties

Property code	Value	Unit	Source
log10ws	5.74		Crippen Method
logp	6.365		Crippen Method
rinpol	1781.00		NIST Webbook
rinpol	1777.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527838&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/38-840-7/Sorbitol-6-methyl-TMS.pdf>

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