

1,4:3,6-Dianhydroglucitol, TMS

Inchi: InChI=1S/C12H26O4Si2/c1-17(2,3)15-9-7-13-12-10(8-14-11(9)12)16-18(4,5)6/h9-12H,7-
InchiKey: LJFXZWTUMDMOLO-WRWGMCAJSA-N
Formula: C12H26O4Si2
SMILES: C[Si](C)(C)OC1COC2C(O[Si](C)(C)C)COC12
Mol. weight [g/mol]: 290.50

Physical Properties

Property code	Value	Unit	Source
log10ws	2.47		Crippen Method
logp	2.224		Crippen Method
rinpol	1523.00		NIST Webbook
rinpol	1523.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R74127&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/48-131-3/1-4-3-6-Dianhydroglucitol-TMS.pdf>

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