

«beta»-2-Deoxy-D-glucose, pyranose, TMS

Inchi: InChI=1S/C17H42O5Si4/c1-23(2,3)19-14-13-15(20-24(4,5)6)18-17(22-26(10,11)12)16(14,15)
InchiKey: VXXVAICYOCQQNP-LTIDMASMSA-N
Formula: C17H42O5Si4
SMILES: C[Si](C)(C)OC1CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)O1
Mol. weight [g/mol]: 438.85

Physical Properties

Property code	Value	Unit	Source
log10ws	4.09		Crippen Method
logp	5.202		Crippen Method
rinpol	1818.00		NIST Webbook
rinpol	1818.00		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=R440845&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/34-905-9/beta-2-Deoxy-D-glucose-pyranose-TMS.pdf>

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