

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

Inchi: InChI=1S/C18H44O5Si4/c1-24(2,3)19-14-16-18(23-27(10,11)12)15(21-25(4,5)6)13-17(20)
InchiKey: DRXHZYOBMYWXSIXLAORIBOSA-N
Formula: C18H44O5Si4
SMILES: C[Si](C)(C)OCC1OC(O[Si](C)(C)C)CC(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 452.88

Physical Properties

Property code	Value	Unit	Source
log10ws	4.17		Crippen Method
logp	5.245		Crippen Method
rinpol	1747.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R440578&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/59-837-8/alpha-2-Deoxy-D-glucose-pyranose-TMS.pdf>

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