

1,4-Anhydrolyxitol, TMS

Inchi: InChI=1S/C14H34O4Si3/c1-19(2,3)16-11-12-14(18-21(7,8)9)13(10-15-12)17-20(4,5)6/h1
InchiKey: HPYHSSSIJAXFKF-RDBSUJKOSA-N
Formula: C14H34O4Si3
SMILES: C[Si](C)(C)OCC1OCC(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 350.67

Physical Properties

Property code	Value	Unit	Source
log10ws	3.59		Crippen Method
logp	3.677		Crippen Method
rinpol	1600.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R74177&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/54-071-3/1-4-Anhydrolyxitol-TMS.pdf>

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