

3-Deoxy-xylo-hexonic acid, 1,4-lactone, TMS

Inchi: InChI=1S/C15H34O5Si3/c1-21(2,3)17-11-14(20-23(7,8)9)12-10-13(15(16)18-12)19-22(4,5)
InchiKey: VULQXPQZKLTTKL-RFHWWMCGSA-N
Formula: C15H34O5Si3
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C1CC(O[Si](C)(C)C)C(=O)O1
Mol. weight [g/mol]: 378.68

Physical Properties

Property code	Value	Unit	Source
log10ws	3.39		Crippen Method
logp	3.594		Crippen Method
rinpol	1802.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R101401&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

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