

3-Deoxy-2C-(hydroxymethyl)threo-pentonic acid lactone, TMS

Inchi: InChI=1S/C17H36O5Si2/c1-16(2,3)22-17(10-11-19-23(4,5)6)12-14(21-15(17)18)13-20-2
InchiKey: VXRFBXFUZNGKOI-PBHICJAKSA-N
Formula: C17H36O5Si2
SMILES: CC(C)(C)OC1(CCO[Si](C)(C)C)CC(CO[Si](C)(C)C)OC1=O
Mol. weight [g/mol]: 376.64

Physical Properties

Property code	Value	Unit	Source
log10ws	0.60		Crippen Method
logp	3.949		Crippen Method
rinpol	1718.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R391392&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/51-639-6/3-Deoxy-2C-hydroxymethyl-threo-pentonic-acid-lactone-TMS.pdf>

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