2-Deoxytetrono-1,4-lactone, mono-TMS

Other names: 2-Deoxytetronic acid, 1,4-lactone, TMS
Inchi: InChI=1S/C7H14O3Si/c1-11(2,3)10-6-4-7(8)9-5-6/h6H,4-5H2,1-3H3
InchiKey: MWWSTXOEDHCEKT-UHFFFAOYSA-N
Formula: C7H14O3Si
SMILES: C[Si](C)(C)OC1COC(=O)C1
Mol. weight [g/mol]: 174.27

Physical Properties

Property code	Value	Unit	Source
log10ws	1.24		Crippen Method
logp	1.153		Crippen Method
rinpol	1216.00		NIST Webbook
rinpol	1223.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R51311&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices