3-Deoxytetronic acid, TMS

Inchi: InChI=1S/C7H14O2Si/c1-10(2,3)9-7-5-4-6-8-7/h5H,4,6H2,1-3H3
InchiKey: ROCZJWMPGISRQB-UHFFFAOYSA-N
Formula: C7H14O2Si
SMILES: C[Si](C)(C)OC1=CCCO1
Mol. weight [g/mol]: 158.27

Physical Properties

Property code	Value	Unit	Source
log10ws	0.28		Crippen Method
logp	2.100		Crippen Method
rinpol	1460.00		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=R594175&Units=SI

Legend

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