

2-C-Methylribonic acid, 1,4-lactone, TMS

Inchi: InChI=1S/C15H34O5Si3/c1-15(20-23(8,9)10)13(19-22(5,6)7)12(18-14(15)16)11-17-21(2,3)
InchiKey: KOEYIGNFJQAGJP-YDHLFZDLSA-N
Formula: C15H34O5Si3
SMILES: CC1(O[Si](C)(C)C)C(=O)OC(CO[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 378.68

Physical Properties

Property code	Value	Unit	Source
log10ws	3.39		Crippen Method
logp	3.594		Crippen Method
rinpol	1657.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R487651&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/49-261-8/2-C-Methylribonic-acid-1-4-lactone-TMS.pdf>

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