

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

Other names:	2C-Methylarabinonic acid 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,
InchiKey:	KOEYIGNFJQAGJP-IPYPFGDCSA-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	1653.00		NIST Webbook
rinpol	1654.00		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=R100824&Units=SI

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/42-010-3/2-C-Methylarabinonic-acid-1-4-lactone-TMS.pdf>

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