

D-Ribo-Hexonic acid, 3-deoxy-2,5,6-tris-O-(trimethylsilyl)-, lactone

Other names:	3-Deoxy-ribo-hexonic acid, 1,4-lactone, (3TMS)- 3-Deoxy-ribo-hexonic acid, 1,4-lactone, TMS
Inchi:	InChI=1S/C15H34O5Si3/c1-21(2,3)17-11-14(20-23(7,8)9)12-10-13(15(16)18-12)19-22(4,
InchiKey:	VULQXPQZKLTTKL-UHFFFAOYSA-N
Formula:	C15H34O5Si3
SMILES:	C[Si](C)(C)OCC(O[Si](C)(C)C)C1CC(O[Si](C)(C)C)C(=O)O1
Mol. weight [g/mol]:	378.68
CAS:	55570-78-0

Physical Properties

Property code	Value	Unit	Source
log10ws	3.39		Crippen Method
logp	3.594		Crippen Method
rinpol	1791.00		NIST Webbook
rinpol	1791.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55570780&Units=SI

Legend

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

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