

3-Hydroxyadipic acid, lacton, TMS

Other names:	3-Hydroxyadipic acid, lactone, mono-TMS
Inchi:	InChI=1S/C9H16O4Si/c1-14(2,3)13-9(11)6-7-4-5-8(10)12-7/h7H,4-6H2,1-3H3
InchiKey:	RASUFFJSOATALI-UHFFFAOYSA-N
Formula:	C9H16O4Si
SMILES:	C[Si](C)(C)OC(=O)CC1CCC(=O)O1
Mol. weight [g/mol]:	216.31

Physical Properties

Property code	Value	Unit	Source
log10ws	0.63		Crippen Method
logp	1.460		Crippen Method
rinpol	1493.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1493.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R164239&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/44-645-7/3-Hydroxyadipic-acid-lacton-TMS.pdf>

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