

D-Glucuronolactone, TMS # 1

Other names:	GLUCURONIC ACID-E-LACTONE 3TMS-1
Inchi:	InChI=1S/C15H32O6Si3/c1-22(2,3)19-11(10-16)12-13(20-23(4,5)6)14(15(17)18-12)21-2
InchiKey:	NGXKKSIAXZQKDH-ZXCYLJYSA-N
Formula:	C15H32O6Si3
SMILES:	C[Si](C)(C)OC(C=O)C1OC(=O)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]:	392.67

Physical Properties

Property code	Value	Unit	Source
log10ws	4.00		Crippen Method
logp	2.771		Crippen Method
rinpol	1899.90		NIST Webbook
rinpol	1913.00		NIST Webbook
rinpol	1899.90		NIST Webbook
rinpol	1913.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R400798&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/113-566-8/D-Glucuronolactone-TMS-1.pdf>

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