

Gluconic acid lactone, TMS # 2

Other names:	GLUCONIC ACID LACTONE 4TMS-2 Glucono-1,5-lactone, TMS # 2
Inchi:	InChI=1S/C18H42O6Si4/c1-25(2,3)20-13-14-15(22-26(4,5)6)16(23-27(7,8)9)17(18(19)21
InchiKey:	VNGTZLYNGGLPIZ-NXOAAHMSSA-N
Formula:	C18H42O6Si4
SMILES:	C[Si](C)(C)OCC1OC(=O)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]:	466.86

Physical Properties

Property code	Value	Unit	Source
log10ws	4.89		Crippen Method
logp	4.424		Crippen Method
rinpol	1923.00		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1923.00		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=R400887&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/28-451-0/Gluconic-acid-lactone-TMS-2.pdf>

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