

Gulonic acid, 2,3,5,6-tetrakis-O-(trimethylsilyl)-, lactone

Other names:

Gulonic acid, 1,4-lactone, (4TMS)-

Gulonic acid, 1,4-lactone, TMS

Gulonic acid, «gamma»-lactone, 4tms derivavative

Inchi: InChI=1S/C18H42O6Si4/c1-25(2,3)20-13-14(22-26(4,5)6)15-16(23-27(7,8)9)17(18(19)21

InchiKey: FTOCXQVQZOFUDF-BACDZXNISA-N

Formula: C18H42O6Si4

SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C1OC(=O)C(O[Si](C)(C)C)C1O[Si](C)(C)C

Mol. weight [g/mol]: 466.86

CAS: 55528-75-1

Physical Properties

Property code	Value	Unit	Source
log10ws	4.89		Crippen Method
logp	4.424		Crippen Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C55528751&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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/66-675-0/Gulonic-acid-2-3-5-6-tetrakis-O-trimethylsilyl-lactone.pdf>

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