

Xylonic acid, 1,4-lactone, TMS

Inchi: InChI=1S/C14H32O5Si3/c1-20(2,3)16-10-11-12(18-21(4,5)6)13(14(15)17-11)19-22(7,8)9
InchiKey: RJMKTJPGOITYTQZ-XQQFMLRXSA-N
Formula: C14H32O5Si3
SMILES: C[Si](C)(C)OCC1OC(=O)C(O[Si](C)(C)C)C1O[Si](C)(C)C
Mol. weight [g/mol]: 364.66

Physical Properties

Property code	Value	Unit	Source
log10ws	3.81		Crippen Method
logp	3.204		Crippen Method
rinpol	1665.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R487735&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/68-597-5/Xylonic-acid-1-4-lactone-TMS.pdf>

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