

Lyxonic acid, «gamma»-lactone, bis-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: RJMKTJPGOIYTQZ-JHJVBTASA-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
logp	3.203		Crippen Method
rinpol	1759.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1759.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R573618&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/53-842-8/Lyxonic-acid-gamma-lactone-bis-TMS.pdf>

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