

ISOCITRIC LACTONE acid, BIS(TRIMETHYLSILYL) ester

Other names: Isocitric lactone acid, bis(trimethylsilyl) ester

Isocitric acid lactone, bis(trimethylsilyl) ester

Lactoisocitric acid, TMS

Isocitric acid lactone, 2tms derivative

Inchi: InChI=1S/C12H22O6Si2/c1-19(2,3)17-11(14)8-7-9(13)16-10(8)12(15)18-20(4,5)6/h8,10H

InchiKey: IBEFDHMMOJYHKQ-UHFFFAOYSA-N

Formula: C12H22O6Si2

SMILES: C[Si](C)(C)OC(=O)C1CC(=O)OC1C(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 318.47

Physical Properties

Property code	Value	Unit	Source
logp	1.674		Crippen Method
rinpol	1710.40		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C65143626&Units=SI>

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

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

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/17-249-7/ISOCITRIC-LACTONE-acid-BIS-TRIMETHYLSILYL-ester.pdf>

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