

Isocitric acid lactone, bis(tert-butyldimethylsilyl) ester

Other names: Isocitric acid lactone, 2tbdms derivative
Inchi: InChI=1S/C18H34O6Si2/c1-17(2,3)25(7,8)23-15(20)12-11-13(19)22-14(12)16(21)24-26(21)
InchiKey: ZHXYTSISPDQOGD-UHFFFAOYSA-N
Formula: C18H34O6Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)C1CC(=O)OC1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 402.63

Physical Properties

Property code	Value	Unit	Source
log10ws	0.19		Crippen Method
logp	4.015		Crippen Method
rinpol	2161.90		NIST Webbook
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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=U352442&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/88-973-5/Isocitric-acid-lactone-bis-tert-butyldimethylsilyl-ester.pdf>

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