

threo-Hex-2-enono-1,4-lactone, TMS

Inchi: InChI=1S/C18H40O6Si4/c1-25(2,3)20-13-14(22-26(4,5)6)16-15(19)17(23-27(7,8)9)18(21)
InchiKey: GXBFYJHYGZGPQB-ZBFHGGJFSA-N
Formula: C18H40O6Si4
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C1OC(O[Si](C)(C)C)=C(O[Si](C)(C)C)C1=O
Mol. weight [g/mol]: 464.85

Physical Properties

Property code	Value	Unit	Source
log10ws	4.27		Crippen Method
logp	4.898		Crippen Method
rinpol	1980.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R307238&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.cheméo.com/cid/34-918-5/threo-Hex-2-enono-1-4-lactone-TMS.pdf>

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