

isoascorbic acid, TMS

Inchi: InChI=1S/C19H42O5Si4/c1-25(2,3)21-14-17(22-26(4,5)6)15-13-16(20)19(24-28(10,11)12)
InchiKey: GQZTXFSFUMBCKP-UHFFFAOYSA-N
Formula: C19H42O5Si4
SMILES: C[Si](C)(C)OCC(O[Si](C)(C)C)C1CC(=O)C(O[Si](C)(C)C)=C1O[Si](C)(C)C
Mol. weight [g/mol]: 462.88

Physical Properties

Property code	Value	Unit	Source
log10ws	3.78		Crippen Method
logp	5.562		Crippen Method
rinpol	1957.40		NIST Webbook
rinpol	1957.40		NIST Webbook
rinpol	2002.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R241653&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.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.chemeo.com/cid/56-843-4/isoascorbic-acid-TMS.pdf>

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