

Quinic acid, TMS

Other names: QUINIC ACID (5TMS)
Inchi: InChI=1S/C22H52O6Si5/c1-29(2,3)24-18-16-22(28-33(13,14)15,21(23)27-32(10,11)12)1
InchiKey: DBCLHKSGLLGXOV-BPBCIEFSSA-N
Formula: C22H52O6Si5
SMILES: C[Si](C)(C)OC(=O)C1(O[Si](C)(C)C)CC(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 553.07

Physical Properties

Property code	Value	Unit	Source
log10ws	5.16		Crippen Method
logp	6.409		Crippen Method
rinpol	1853.80		NIST Webbook
rinpol	1854.90		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1918.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R14911&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/47-639-1/Quinic-acid-TMS.pdf>

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