

Tartronic acid, TMS # 4

Inchi: InChI=1S/C12H28O5Si3/c1-18(2,3)15-10(11(13)16-19(4,5)6)12(14)17-20(7,8)9/h10H,1-9
InchiKey: FVBGDMUSQDIQPK-UHFFFAOYSA-N
Formula: C₁₂H₂₈O₅Si₃
SMILES: C[Si](C)(C)OC(=O)C(O[Si](C)(C)C)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 336.60

Physical Properties

Property code	Value	Unit	Source
log10ws	4.08		Crippen Method
logp	2.963		Crippen Method
rinpol	1661.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R401642&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/114-961-8/Tartronic-acid-TMS-4.pdf>

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