

Tetronic acid, TMS

Inchi: InChI=1S/C7H12O3Si/c1-11(2,3)10-7-5-4-6(8)9-7/h4-5,7H,1-3H3
InchiKey: OLWNNFLDXJEWQF-UHFFFAOYSA-N
Formula: C7H12O3Si
SMILES: C[Si](C)(C)OC1C=CC(=O)O1
Mol. weight [g/mol]: 172.25

Physical Properties

Property code	Value	Unit	Source
log10ws	0.89		Crippen Method
logp	1.277		Crippen Method
rinpol	1366.00		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=R401657&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.cheméo.com/cid/21-069-2/Tetronic-acid-TMS.pdf>

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