

5-Hydroxymethyl-2-furoic acid, monoTMS

Inchi: InChI=1S/C9H14O4Si/c1-14(2,3)13-9(11)8-5-4-7(6-10)12-8/h4-5,10H,6H2,1-3H3
InchiKey: HYDLFRRTORFTFZ-UHFFFAOYSA-N
Formula: C9H14O4Si
SMILES: C[Si](C)(C)OC(=O)c1ccc(CO)o1
Mol. weight [g/mol]: 214.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.48		Crippen Method
logp	1.764		Crippen Method
rinpol	1554.00		NIST Webbook
rinpol	1554.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R273239&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/57-509-4/5-Hydroxymethyl-2-furoic-acid-monoTMS.pdf>

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