

Aceburic acid, TMS

Inchi: InChI=1S/C9H18O4Si/c1-8(10)12-7-5-6-9(11)13-14(2,3)4/h5-7H2,1-4H3
InchiKey: SGAHIRVSGAMDSV-UHFFFAOYSA-N
Formula: C9H18O4Si
SMILES: CC(=O)OCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 218.32
CAS: 959051-58-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.63		Crippen Method
logp	1.708		Crippen Method
rinpol	1173.80		NIST Webbook
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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=C959051582&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.chemeo.com/cid/98-856-4/Aceburic-acid-TMS.pdf>

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