Succinic acid, monoethyl ester-, (TMS)

Inchi: InChI=1S/C9H18O4Si/c1-5-12-8(10)6-7-9(11)13-14(2,3)4/h5-7H2,1-4H3
InchiKey: UXHNYNXKXHRDRI-UHFFFAOYSA-N
Formula: C9H18O4Si
SMILES: CCOC(=O)CCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 218.32
CAS: 959313-61-2

Physical Properties

Property code	Value	Unit	Source
log10ws	0.63		Crippen Method
logp	1.708		Crippen Method
rinpol	1250.60		NIST Webbook
rinpol	1250.60		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C959313612&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices