Succinylacetone, TBDMS # 3

Inchi: InChI=1S/C19H38O4Si2/c1-15(20)14-16(22-24(8,9)18(2,3)4)12-13-17(21)23-25(10,11)19

InchiKey: AFAGHMMNXDARQM-UHFFFAOYSA-N

Formula: C19H38O4Si2

SMILES: CC(=O)CC(=CCC(=O)O[Si](C)(C)C(C)(C)C)O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]: 386.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.46		Crippen Method
logp	5.810		Crippen Method
rinpol	1817.00		NIST Webbook
rinpol	1825.00		NIST Webbook
rinpol	1817.00		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=R565023&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices