Jasmonic acid, TBDMS

Inchi: InChI=1S/C17H30O3Si/c1-7-8-9-10-13-14(11-12-15(13)18)16(19)20-21(5,6)17(2,3)4/h8-
InchiKey: NCZMPTIYORNFDE-NYCDYWJRSA-N
Formula: C17H30O3Si
SMILES: CCC=CCC1C(=O)CCC1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 310.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	4.486		Crippen Method
rinpol	1984.00		NIST Webbook
rinpol	1984.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R282609&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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