3-Butenoic acid, trimethylsilyl ester

Other names: 3-Butenoic acid, tms derivative
Inchi: InChI=1S/C7H14O2Si/c1-5-6-7(8)9-10(2,3)4/h5H,1,6H2,2-4H3
InchiKey: NJLWVYLLRXIFHK-UHFFFAOYSA-N
Formula: C7H14O2Si
SMILES: C=CCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 158.27

Physical Properties

Property code	Value	Unit	Source
log10ws	0.48		Crippen Method
logp	1.941		Crippen Method
rinpol	874.10		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=U333860&Units=SI

Legend

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