3-Butenoic acid, tert-butyldimethylsilyl ester

Other names:	tert-Butyl(dimethyl)silyl but-3-enoate
	3-Butenoic acid, tbdms derivative
Inchi:	InChI=1S/C10H20O2Si/c1-7-8-9(11)12-13(5,6)10(2,3)4/h7H,1,8H2,2-6H3
InchiKey:	ACAPMVQJXTXROZ-UHFFFAOYSA-N
Formula:	C10H20O2Si
SMILES:	C=CCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	200.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.78		Crippen Method
logp	3.111		Crippen Method
rinpol	1088.60		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333147&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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