

Geranic acid TMS

Inchi:	InChI=1S/C13H24O2Si/c1-11(2)8-7-9-12(3)10-13(14)15-16(4,5)6/h8,10H,7,9H2,1-6H3/b
InchiKey:	DJMORKDGMCSRBR-ZRDIBKRKSA-N
Formula:	C13H24O2Si
SMILES:	CC(C)=CCCC(C)=CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	240.41
CAS:	97779-61-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.88		Crippen Method
logp	4.057		Crippen Method
rinpol	1447.60		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97779618&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/118-750-8/Geranic-acid-TMS.pdf>

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