

Valerenic acid, TMS

Inchi: InChI=1S/C18H30O2Si/c1-12-7-9-15(17-13(2)8-10-16(12)17)11-14(3)18(19)20-21(4,5)6/
InchiKey: HMLOHZYWWAHRQD-SDNWHVVSQSA-N
Formula: C18H30O2Si
SMILES: CC(=CC1CCC(C)C2CCC(C)=C12)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 306.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.04		Crippen Method
logp	5.083		Crippen Method
rinpol	1883.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U414251&Units=SI>

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/97-483-9/Valerenic-acid-TMS.pdf>

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