

6-[12(Z)-Nonadecenyl]salicylic acid (2TMS)

Inchi: InChI=1S/C32H58O3Si2/c1-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-24-26-29-2
InchiKey: XKABAQWKVSFZDL-YPKPFQOOSA-N
Formula: C32H58O3Si2
SMILES: CCCCCC=CCCCCCCCCCCCc1cccc(O[Si](C)(C)C)c1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 546.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.38		Crippen Method
logp	10.862		Crippen Method
rinpol	3226.30		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U414067&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/72-055-1/6-12-Z-Nonadecenyl-salicylic-acid-2TMS.pdf>

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