

Geranyl (E)-p-coumarate, mono-TMS

Inchi: InChI=1S/C22H32O3Si/c1-18(2)8-7-9-19(3)16-17-24-22(23)15-12-20-10-13-21(14-11-20)
InchiKey: MZPYHALLWWGKOP-PZGOMQMCSA-N
Formula: C22H32O3Si
SMILES: CC(C)=CCCC(C)=CCOC(=O)C=Cc1ccc(O[Si](C)(C)C)cc1
Mol. weight [g/mol]: 372.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.48		Crippen Method
logp	6.149		Crippen Method
rinpol	2653.00		NIST Webbook
rinpol	2663.00		NIST Webbook

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=R55917&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/32-695-5/Geranyl-E-p-coumarate-mono-TMS.pdf>

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