

Benzyl (E)-caffeate, TMS

Inchi: InChI=1S/C22H30O4Si2/c1-27(2,3)25-20-14-12-18(16-21(20)26-28(4,5)6)13-15-22(23)24
InchiKey: SDXLQJAPPVWFDV-FYWRMAATSA-N
Formula: C22H30O4Si2
SMILES: C[Si](C)(C)Oc1ccc(C=CC(=O)OCc2ccccc2)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 414.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	5.871		Crippen Method
rinpol	2679.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R173134&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/121-080-8/Benzyl-E-caffeate-TMS.pdf>

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