

2-Phenylethyl (E)-3-acetylcaffeate, TMS

Inchi:	InChI=1S/C22H26O5Si/c1-17(23)26-21-16-19(10-12-20(21)27-28(2,3)4)11-13-22(24)25-
InchiKey:	JLGGKGJZXSCANR-ACCUITESSA-N
Formula:	C22H26O5Si
SMILES:	CC(=O)Oc1cc(C=CC(=O)OCCc2ccccc2)ccc1O[Si](C)(C)C
Mol. weight [g/mol]:	398.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.35		Crippen Method
logp	4.625		Crippen Method
rinpol	2844.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R173025&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/84-608-4/2-Phenylethyl-E-3-acetylcaffeate-TMS.pdf>

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