

Coumaryl (E)-cinnamate, mono-TMS

Inchi: InChI=1S/C21H24O3Si/c1-25(2,3)24-20-14-11-19(12-15-20)10-7-17-23-21(22)16-13-18-
InchiKey: RURNVJNXWGSXQM-NJKRNUQASA-N
Formula: C21H24O3Si
SMILES: C[Si](C)(C)Oc1ccc(C=CCOC(=O)C=Cc2ccccc2)cc1
Mol. weight [g/mol]: 352.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	5.170		Crippen Method
rinpol	2770.00		NIST Webbook
rinpol	2770.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R55743&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/84-725-4/Coumaryl-E-cinnamate-mono-TMS.pdf>

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