

Hydrocinnamyl (E)-isoferulate, TMS

Inchi: InChI=1S/C22H28O4Si/c1-24-20-14-12-19(17-21(20)26-27(2,3)4)13-15-22(23)25-16-8-1
InchiKey: FJJTTWOOMQXNLK-FYWRMAATSA-N
Formula: C22H28O4Si
SMILES: COc1ccc(C=CC(=O)OCCc2ccccc2)cc1O[Si](C)(C)C
Mol. weight [g/mol]: 384.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.57		Crippen Method
logp	5.098		Crippen Method
rinpol	2813.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R42326&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.cheméo.com/cid/17-393-7/Hydrocinnamyl-E-isoferulate-TMS.pdf>

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