

trans-2,4-Dimethoxycinnamic acid, trimethylsilyl ester

Other names: 2,4-Dimethoxycinnamic acid, (e)-, tms derivative
Inchi: InChI=1S/C14H20O4Si/c1-16-12-8-6-11(13(10-12)17-2)7-9-14(15)18-19(3,4)5/h6-10H,1-
InchiKey: CODYUIBECSYZDZ-VQHVLOKHSA-N
Formula: C14H20O4Si
SMILES: COc1ccc(C=CC(=O)O[Si](C)(C)C)c(OC)c1
Mol. weight [g/mol]: 280.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.12		Crippen Method
logp	3.095		Crippen Method
rinpol	2061.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352418&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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