

cis-Caffeic acid, 3TMS

Inchi: InChI=1S/C18H32O4Si3/c1-23(2,3)20-16-12-10-15(14-17(16)21-24(4,5)6)11-13-18(19)2
InchiKey: MBIYCWDFSLHMSI-QBFSEMIESA-N
Formula: C18H32O4Si3
SMILES: C[Si](C)(C)OC(=O)C=Cc1ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 396.70

Physical Properties

Property code	Value	Unit	Source
log10ws	1.10		Crippen Method
logp	5.505		Crippen Method
rinpol	2101.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R576979&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/55-246-8/cis-Caffeic-acid-3TMS.pdf>

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