

trans-Ferulic acid, 2TMS

Inchi: InChI=1S/C16H26O4Si2/c1-18-15-12-13(8-10-14(15)19-21(2,3)4)9-11-16(17)20-22(5,6)7
InchiKey: UQBSUVIBJIXFQT-PKQBQFBNSA-N
Formula: C16H26O4Si2
SMILES: COc1cc(C=CC(=O)O[Si](C)(C)C)ccc1O[Si](C)(C)C
Mol. weight [g/mol]: 338.55

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.01		Crippen Method
logp	4.300		Crippen Method
rinpol	2058.00		NIST Webbook
rinpol	2058.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R577249&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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<https://www.cheméo.com/cid/36-997-6/trans-Ferulic-acid-2TMS.pdf>

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