

Cinnamic acid, 4-(t-butyldimethylsilyloxy)-, t-butyldimethylsilyl ester

Other names: 4-Hydroxycinnamic acid, TBDMS
p-Coumaric acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester

Inchi: InChI=1S/C21H36O3Si2/c1-20(2,3)25(7,8)23-18-14-11-17(12-15-18)13-16-19(22)24-26(27,28)29

InchiKey: NZONQIYPUOMCTJ-DTQAZKPQSA-N

Formula: C₂₁H₃₆O₃Si₂

SMILES: CC(C)(C)[Si](C)(C)OC(=O)C=Cc1ccc(O[Si](C)(C)C(C)(C)C)cc1

Mol. weight [g/mol]: 392.68

CAS: 254985-03-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	6.632		Crippen Method
rinpol	2452.10		NIST Webbook
rinpol	2462.00		NIST Webbook
rinpol	2452.10		NIST Webbook
rinpol	2462.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C254985030&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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