

trans-2-Hydroxycinnamic acid, tert-butyl dimethylsilyl ether, tert-butyl dimethylsilyl ester

Other names: O-coumaric acid, 2-hydroxy derivative
InChI: InChI=1S/C21H36O3Si2/c1-20(2,3)25(7,8)23-18-14-12-11-13-17(18)15-16-19(22)24-26(27,28)29
InchiKey: KEJAOBNCADPMEY-FOCLMDBBSA-N
Formula: C21H36O3Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)C=Cc1ccccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 392.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	6.632		Crippen Method
rinpol	2287.60		NIST Webbook
rinpol	2287.60		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U352488&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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/122-923-1/trans-2-Hydroxycinnamic-acid-tert-butyl dimethylsilyl ether-tert-butyl dimethylsilyl ester>

Generated by Cheméo on 2024-04-29 11:22:56.085186964 +0000 UTC m=+16679025.005764276.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.