

trans-3-Hydroxycinnamic acid, tert-butyl dimethylsilyl ether, tert-butyl dimethylsilyl ester

Other names: 3-Coumaric acid, TBDMS
Inchi: InChI=1S/C21H36O3Si2/c1-20(2,3)25(7,8)23-18-13-11-12-17(16-18)14-15-19(22)24-26(27,28)29
InchiKey: AXVWZAUGUOJORB-CCEZHUSRSA-N
Formula: C21H36O3Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)C=Cc1cccc(O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]: 392.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.40		Crippen Method
logp	6.632		Crippen Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U364370&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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