

3,4-Dihydroxyhydrocinnamic acid, O,O-bis-(tert-butyl dimethylsilyl)-, tert-butyl dimethylsilyl ester

Other names: tert-Butyl(dimethyl)silyl 3,4-dihydroxyhydrocinnamic acid, 3tbodms derivative

Inchi:	InChI=1S/C27H52O4Si3/c1-25(2,3)32(10,11)29-22-18-16-21(20-23(22)30-33(12,13)26(4
InchiKey:	JMHNVFIWSDJNGF-UHFFFAOYSA-N
Formula:	C27H52O4Si3
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)CCc1ccc(O[Si](C)(C)C(C)(C)C)c(O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]:	524.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	8.936		Crippen Method
rinpol	2628.70		NIST Webbook
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Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U332777&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices

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