

Dihydrochalcone, 2',6'-dihydroxy-4'-methoxy, bis-TMS

Other names:	Dihydrochalcone, 2',6'-dihydroxy-4'-methoxy, TMS
Inchi:	InChI=1S/C22H32O4Si2/c1-24-18-15-21(25-27(2,3)4)19(22(16-18)26-28(5,6)7)13-14-20
InchiKey:	CZLQSZKEHUXCSU-UHFFFAOYSA-N
Formula:	C22H32O4Si2
SMILES:	COc1cc(O[Si](C)(C)C)c(CCC(=O)c2ccccc2)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]:	416.66

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	5.938		Crippen Method
rinpol	2388.00		NIST Webbook
rinpol	2378.00		NIST Webbook
rinpol	2378.00		NIST Webbook
rinpol	2388.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R46338&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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/96-033-9/Dihydrochalcone-2-6-dihydroxy-4-methoxy-bis-TMS.pdf>

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