

Chalcone, 2',4,4',6'-tetrahydroxy, TMS

Other names:	Chalcone, 2',4',6',4-tetrahydroxy, tetrakis-TMS
Inchi:	InChI=1S/C27H44O5Si4/c1-33(2,3)29-22-15-13-21(14-16-22)25(28)18-17-24-26(31-35(7
InchiKey:	CKVYKENYJLBJLV-ISLYRVAYSA-N
Formula:	C27H44O5Si4
SMILES:	C[Si](C)(C)Oc1ccc(C(=O)C=Cc2c(O[Si](C)(C)C)cc(O[Si](C)(C)C)cc2O[Si](C)(C)C)cc1
Mol. weight [g/mol]:	560.98

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.22		Crippen Method
logp	8.438		Crippen Method
rinpol	2862.00		NIST Webbook
rinpol	2854.00		NIST Webbook
rinpol	2854.00		NIST Webbook
rinpol	2862.00		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=R46267&Units=SI

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/113-073-5/Chalcone-2-4-4-6-tetrahydroxy-TMS.pdf>

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