

Flavanone, 3,5,7-trihydroxy, TMS

Other names:	Flavanone, 3,5,7-trihydroxy, tris-TMS
Inchi:	InChI=1S/C24H36O5Si3/c1-30(2,3)27-18-15-19-21(20(16-18)28-31(4,5)6)22(25)24(29-30)3
InchiKey:	AONLCEUOCFEYLB-UHFFFAOYSA-N
Formula:	C ₂₄ H ₃₆ O ₅ Si ₃
SMILES:	C[Si](C)(C)Oc1cc2c(c(O[Si](C)(C)C)c1)C(=O)C(O[Si](C)(C)C)C(c1cccc1)O2
Mol. weight [g/mol]:	488.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.74		Crippen Method
logp	6.651		Crippen Method
rinpol	2573.00		NIST Webbook
rinpol	2583.00		NIST Webbook
rinpol	2577.00		NIST Webbook
rinpol	2577.00		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=R46356&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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<https://www.cheméo.com/cid/36-691-5/Flavanone-3-5-7-trihydroxy-TMS.pdf>

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