

4H-1-Benzopyran-4-one, 2-[3,4-bis[(trimethylsilyl)oxy]phenyl]-3,5,7-tris[(tri

Other names:	Flavone, 3,3',4',5,7-pentahydroxy, TMS Quercetin, (5TMS) Flavone, 3,3',4',5,7-pentakis(trimethylsiloxy)- Quercetin, TMS Quercetin, penta-TMS Quercetin, 5tms derivative
Inchi:	InChI=1S/C30H50O7Si5/c1-38(2,3)33-22-19-25-27(26(20-22)36-41(10,11)12)28(31)30(3
InchiKey:	VISLTJDFZRIFEA-UHFFFAOYSA-N
Formula:	C30H50O7Si5
SMILES:	C[Si](C)(C)Oc1cc(O[Si](C)(C)C)c2c(=O)c(O[Si](C)(C)C)c(-c3ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c3)cc1
Mol. weight [g/mol]:	663.14
CAS:	4067-66-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.07		Crippen Method
logp	9.528		Crippen Method
rinpol	3219.70		NIST Webbook
rinpol	3174.60		NIST Webbook
rinpol	3171.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4067667&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/46-116-2/4H-1-Benzopyran-4-one-2-3-4-bis-trimethylsilyl-oxy-phenyl-3-5-7-tris-trimethyl>

Generated by Cheméo on 2024-04-27 20:14:17.817900576 +0000 UTC m=+16538106.738477896.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.