

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

Other names: Chalcone, 2',4',6'-trihydroxy, tris-TMS
Inchi: InChI=1S/C24H36O4Si3/c1-29(2,3)26-20-17-23(27-30(4,5)6)21(24(18-20)28-31(7,8)9)15
InchiKey: QVGPOKXGZYTABA-FOCLMDBBSA-N
Formula: C24H36O4Si3
SMILES: C[Si](C)(C)Oc1cc(O[Si](C)(C)C)c(C=CC(=O)c2ccccc2)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 472.80

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.21		Crippen Method
logp	7.224		Crippen Method
rinpol	2501.00		NIST Webbook
rinpol	2511.00		NIST Webbook
rinpol	2499.00		NIST Webbook
rinpol	2501.00		NIST Webbook
rinpol	2499.00		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=R46253&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/119-679-7/Chalcone-2-4-6-trihydroxy-TMS.pdf>

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