

Dihydrochalcone, 2',4',6'-trihydroxy-4-methoxy, TMS

Other names: Dihydrochalcone, 2',4',6'-trihydroxy-4-methoxy, tris-TMS
Inchi: InChI=1S/C25H40O5Si3/c1-27-20-13-11-19(12-14-20)23(26)16-15-22-24(29-32(5,6)7)17
InchiKey: QXANHWYOJHTUGK-UHFFFAOYSA-N
Formula: C₂₅H₄₀O₅Si₃
SMILES: COc1ccc(C(=O)CCc2c(O[Si](C)(C)C)cc(O[Si](C)(C)C)cc2O[Si](C)(C)C)cc1
Mol. weight [g/mol]: 504.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.31		Crippen Method
logp	7.152		Crippen Method
rinpol	2653.00		NIST Webbook
rinpol	2661.00		NIST Webbook
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R46299&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/24-220-0/Dihydrochalcone-2-4-6-trihydroxy-4-methoxy-TMS.pdf>

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