

Flavone, 3,5,7-trihydroxy, tris-TMS

Inchi: InChI=1S/C24H34O5Si3/c1-30(2,3)27-18-15-19-21(20(16-18)28-31(4,5)6)22(25)24(29-30)32
InchiKey: RDCHQJXIQXSZNH-UHFFFAOYSA-N
Formula: C₂₄H₃₄O₅Si₃
SMILES: C[Si](C)(C)Oc1cc(O[Si](C)(C)C)c2c(=O)c(O[Si](C)(C)C)c(-c3ccccc3)oc2c1
Mol. weight [g/mol]: 486.78

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.06		Crippen Method
logp	7.101		Crippen Method
rinpol	2745.00		NIST Webbook
rinpol	2738.00		NIST Webbook
rinpol	2692.00		NIST Webbook
rinpol	2745.00		NIST Webbook
rinpol	2785.00		NIST Webbook
rinpol	2738.00		NIST Webbook
rinpol	2692.00		NIST Webbook
rinpol	2785.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R46235&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/120-132-1/Flavone-3-5-7-trihydroxy-tris-TMS.pdf>

Generated by Cheméo on 2024-04-28 23:24:22.161164237 +0000 UTC m=+16635911.081741549.

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