

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

Inchi: InChI=1S/C21H26O5Si2/c1-27(2,3)25-15-12-16-18(17(13-15)26-28(4,5)6)19(22)20(23)2
InchiKey: XEBOPEAAOAXVHM-UHFFFAOYSA-N
Formula: C21H26O5Si2
SMILES: C[Si](C)(C)Oc1cc(O[Si](C)(C)C)c2c(=O)c(O)c(-c3ccccc3)oc2c1
Mol. weight [g/mol]: 414.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.60		Crippen Method
logp	5.593		Crippen Method
rinpol	2677.00		NIST Webbook
rinpol	2686.00		NIST Webbook
rinpol	2683.00		NIST Webbook
rinpol	2677.00		NIST Webbook
rinpol	2683.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R46221&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/61-833-9/Flavone-3-5-7-trihydroxy-bis-TMS.pdf>

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