

Fisetin, TMS

Inchi: InChI=1S/C27H42O6Si4/c1-34(2,3)30-20-14-15-21-23(18-20)29-26(27(25(21)28)33-37(1
InchiKey: LZIQFUABPZZTFQ-UHFFFAOYSA-N
Formula: C27H42O6Si4
SMILES: C[Si](C)(C)Oc1ccc2c(=O)c(O[Si](C)(C)C)c(-c3ccc(O[Si](C)(C)C)c(O[Si](C)(C)C)c3)oc2c1
Mol. weight [g/mol]: 574.96

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	8.315		Crippen Method
rinpol	3125.40		NIST Webbook
rinpol	3155.90		NIST Webbook
rinpol	3125.40		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=R760&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/115-013-9/Fisetin-TMS.pdf>

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