

Flavone, 5,7-dihydroxy, mono-TMS

Other names:	Chrysin (5,7-dihydroxyflavone), monoTMS
Inchi:	InChI=1S/C18H18O4Si/c1-23(2,3)22-13-9-14(19)18-15(20)11-16(21-17(18)10-13)12-7-5
InchiKey:	KNSJFFBZGDMNLU-UHFFFAOYSA-N
Formula:	C18H18O4Si
SMILES:	C[Si](C)(C)Oc1cc(O)c2c(=O)cc(-c3ccccc3)oc2c1
Mol. weight [g/mol]:	326.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.59		Crippen Method
logp	4.379		Crippen Method
rinpol	2644.00		NIST Webbook
rinpol	2589.00		NIST Webbook
rinpol	2616.00		NIST Webbook
rinpol	2644.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R55903&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.chemeo.com/cid/36-071-3/Flavone-5-7-dihydroxy-mono-TMS.pdf>

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