

Daidzein, TMS

Other names:	DAIDZEIN 2TMS
Inchi:	InChI=1S/C21H26O4Si2/c1-26(2,3)24-16-9-7-15(8-10-16)19-14-23-20-13-17(25-27(4,5)6
InchiKey:	OTTQJFPQFUCPEZ-UHFFFAOYSA-N
Formula:	C21H26O4Si2
SMILES:	<chem>C[Si](C)(C)Oc1ccc(-c2coc3cc(O[Si](C)(C)C)ccc3c2=O)cc1</chem>
Mol. weight [g/mol]:	398.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.05		Crippen Method
logp	5.887		Crippen Method
rinpol	2929.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R570&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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/38-402-3/Daidzein-TMS.pdf>

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