

Dihydrodaidzein (enol) di-4,7-d9-TMS

Inchi: InChI=1S/C21H28O4Si2/c1-26(2,3)24-17-11-12-18-20(13-17)23-14-19(21(18)25-27(4,5))
InchiKey: VAOOQOFSZUUMNJ-UHFFFAOYSA-N
Formula: C21H28O4Si2
SMILES: C[Si](C)(C)OC1=C(c2ccc(O)cc2)COc2cc(O[Si](C)(C)C)ccc21
Mol. weight [g/mol]: 400.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	5.718		Crippen Method
rinpol	2700.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R261444&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/114-466-8/Dihydrodaidzein-enol-di-4-7-d9-TMS.pdf>

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