

Toralactone, TMS

Inchi: InChI=1S/C21H28O5Si2/c1-13-9-14-10-15-11-16(23-2)12-17(25-27(3,4)5)18(15)20(26-2)
InchiKey: LFOLKGBJLPMTQD-UHFFFAOYSA-N
Formula: C21H28O5Si2
SMILES: COc1cc(O[Si](C)(C)C)c2c(O[Si](C)(C)C)c3c(=O)oc(C)cc3cc2c1
Mol. weight [g/mol]: 416.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.85		Crippen Method
logp	5.691		Crippen Method
rinpol	2657.00		NIST Webbook
rinpol	2657.00		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=R158333&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/16-588-2/Toralactone-TMS.pdf>

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