

Pinselin, TMS

Inchi: InChI=1S/C22H28O6Si2/c1-13-11-16-18(17(12-13)28-30(6,7)8)21(23)19-14(26-16)9-10-
InchiKey: CZEWKDBCFXCLLQ-UHFFFAOYSA-N
Formula: C22H28O6Si2
SMILES: COC(=O)c1c(O[Si](C)(C)C)ccc2oc3cc(C)cc(O[Si](C)(C)C)c3c(=O)c12
Mol. weight [g/mol]: 444.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.97		Crippen Method
logp	5.469		Crippen Method
rinpol	2808.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R158308&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/14-980-8/Pinselin-TMS.pdf>

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