Chryso-obtusin, TMS

Inchi: InChI=1S/C22H26O7Si/c1-11-9-12-15(21(27-4)19(11)29-30(6,7)8)18(24)16-13(17(12)23)
InchiKey: UTVRRLPSYHUOSU-UHFFFAOYSA-N
Formula: C22H26O7Si
SMILES: COc1cc2c(c(OC)c1OC)C(=O)c1c(cc(C)c(O[Si](C)(C)C)c1OC)C2=O
Mol. weight [g/mol]: 430.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	4.019		Crippen Method
rinpol	3060.00		NIST Webbook
rinpol	3060.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R158195&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