Isoflupredone, tetra-TMS

Inchi: InChI=1S/C33H59FO5Si4/c1-30-19-17-25(37-41(6,7)8)21-24(30)15-16-27-26-18-20-32(3
InchiKey: AHVIRMXYSRSHLO-MANJPLSISA-N
Formula: C33H59FO5Si4
SMILES: CC12C=CC(O[Si](C)(C)C)=CC1=CCC1C3CCC(O[Si](C)(C)C)(C(=O)CO[Si](C)(C)C)C3(C
Mol. weight [g/mol]: 667.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.33		Crippen Method
logp	9.003		Crippen Method
rinpol	3323.00		NIST Webbook
rinpol	3323.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R558060&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices