Triamcinolone, 11-keto, MO TMS

Inchi: InChI=1S/C33H58FN3O6Si3/c1-30-18-17-24(35-38-3)19-23(30)15-16-25-26-20-29(42-45
InchiKey: RNTGLNFXIJRWIK-JXZVQOGHSA-N
Formula: C33H58FN3O6Si3
SMILES: CON=C1C=CC2(C)C(=C1)CCC1C3CC(O[Si](C)(C)C)C(O[Si](C)(C)C)(C(CO[Si](C)(C)C)=
Mol. weight [g/mol]: 696.09

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.28		Crippen Method
logp	7.706		Crippen Method
rinpol	3348.00		NIST Webbook
rinpol	3348.00		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=R44106&Units=SI

Legend

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