

Tetrahydrodehydrocorticosterone enol-TMS

Inchi: InChI=1S/C27H48O4Si2/c1-26-14-13-19(31-33(6,7)8)15-18(26)9-10-20-21-11-12-22(24)
InchiKey: FHIUFWXLUPHIFD-FVLNIECGSA-N
Formula: C27H48O4Si2
SMILES: CC12CC(=O)C3C(CCC4CC(O[Si](C)(C)C)CCC43C)C1CCC2C(=O)CO[Si](C)(C)C
Mol. weight [g/mol]: 492.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Crippen Method
logp	6.465		Crippen Method
rinpol	3129.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R384146&Units=SI>

Legend

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

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