

Tetrahydrocorticoesterone, MO-TMS # 2

Inchi: InChI=1S/C31H61NO4Si3/c1-30-18-17-23(35-38(7,8)9)19-22(30)13-14-24-25-15-16-26(27,28)31-29-20-21-22-23-24-25-26-27-28-29-30-31
InchiKey: LTUTXXUPIPZWMI-GUPMVVFRSA-N
Formula: C31H61NO4Si3
SMILES: CON=C(CO[Si](C)(C)C)C1CCC2C3CCC4CC(O[Si](C)(C)C)CCC4(C)C3C(O[Si](C)(C)C)C1
Mol. weight [g/mol]: 596.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.57		Crippen Method
logp	8.549		Crippen Method
rinpol	3077.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R527605&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

Latest version available from:

<https://www.chemeo.com/cid/20-398-8/Tetrahydrocorticoesterone-MO-TMS-2.pdf>

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