

16«alpha»-Hydroxy-dehydroepiandrosterone, MO-TMS, # 1

Inchi: InChI=1S/C26H47NO3Si2/c1-25-14-12-19(29-31(4,5)6)16-18(25)10-11-20-21(25)13-15-2
InchiKey: SROWHFXQCGCWEL-NWNDOREWSA-N
Formula: C26H47NO3Si2
SMILES: CON=C1C(O[Si](C)(C)C)CC2C3CC=C4CC(O[Si](C)(C)C)CCC4(C)C3CCC12C
Mol. weight [g/mol]: 477.83

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.27		Cheméo Relay (1.0)
logp	7.002		Crippen Method
rinpol	2805.00		NIST Webbook
rinpol	2805.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R537058&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/37-082-0/16-alpha-Hydroxy-dehydroepiandrosterone-MO-TMS-1.pdf>

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