

2-Methoxyestrone, TMS

Inchi: InChI=1S/C25H40O3Si2/c1-25-14-13-18-19(21(25)11-12-24(25)28-30(6,7)8)10-9-17-15-
InchiKey: CCKVXERFVHVQPN-XDSPWSPCSA-N
Formula: C25H40O3Si2
SMILES: COc1cc2c(cc1O[Si](C)(C)C)CCC1C2CCC2(C)C(O[Si](C)(C)C)=CCC12
Mol. weight [g/mol]: 444.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.22		Crippen Method
logp	7.110		Crippen Method
rinpol	2680.00		NIST Webbook
rinpol	2697.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R525689&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/19-535-7/2-Methoxyestrone-TMS.pdf>

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