Estradiol, VDMS

Inchi: InChI=1S/C26H40O2Si2/c1-8-29(4,5)27-20-11-13-21-19(18-20)10-12-23-22(21)16-17-26
InchiKey: UMKNFDWBBYRMIO-FZPKUJNRSA-N
Formula: C26H40O2Si2
SMILES: C=C[Si](C)(C)Oc1ccc2c(c1)CCC1C2CCC2(C)C(O[Si](C)(C)C=C)CCC12
Mol. weight [g/mol]: 440.77

Physical Properties

Property code	Value	Unit	Source
ie	8.60	eV	Cheméo Relay (1.0)
log10ws	-6.17		Cheméo Relay (1.0)
logp	7.167		Crippen Method
rinpol	2856.00		NIST Webbook
rinpol	2856.00		NIST Webbook
tf	352.07	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R529567&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

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https://www.chemeo.com/cid/54-696-0/Estradiol-VDMS.pdf

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