

Estrone, VDMS

Inchi: InChI=1S/C26H38O2Si2/c1-8-29(4,5)27-20-11-13-21-19(18-20)10-12-23-22(21)16-17-26
InchiKey: QRKQMGCPKPZOOJ-HPUZDQILSA-N
Formula: C26H38O2Si2
SMILES: C=C[Si](C)(C)OC1=CCC2C3CCc4cc(O[Si](C)(C)C=C)ccc4C3CCC12C
Mol. weight [g/mol]: 438.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.82		Crippen Method
logp	7.292		Crippen Method
rinpol	2661.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R529587&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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.cheméo.com/cid/16-197-6/Estrone-VDMS.pdf>

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