

Danazol (2,4-Pregnadien-(2,3-d)isoxazol-17A-ethynyl-17B-ol-TMS

TMS

InChI=1S/C25H35NO2Si/c1-7-25(28-29(4,5)6)13-11-21-19-9-8-18-14-22-17(16-26-27-22)

InchiKey: GYVWITJCAJQCRU-ZEKWSJBJSJSA-N

Formula: C₂₅H₃₅NO₂Si

SMILES: C#CC1(O[Si](C)(C)C)CCC2C3CCC4=Cc5oncc5CC4(C)C3CCC21C

Mol. weight [g/mol]: 409.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.55		Crippen Method
logp	6.080		Crippen Method
rinpol	3111.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R585527&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/114-736-8/Danazol-2-4-Pregnadien-2-3-d-isoxazol-17A-ethynyl-17B-ol-TMS.pdf>

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