

2,4-Pregnadien-(2,3-d)isoxazol-17.alpha.-ethynyl-17-beta-ol-TMS

InChIKey:

InChI=1S/C25H35NO2Si/c1-7-25(28-29(4,5)6)13-11-21-19-9-8-18-14-22-17(16-27-26-22)20-24

VTXNBONLVUSKRW-DWSVNQEMSA-N

Formula:

C₂₅H₃₅NO₂Si

SMILES:

C#C[C@]1(O[Si](C)(C)C)CCC2C3CCC4=Cc5nocc5C[C@]4(C)C3CC[C@@]21C

Mol. weight [g/mol]:

409.65

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.94		Cheméo Relay (1.0)
logp	6.080		Crippen Method
tf	431.42	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?Str2File=R321972>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

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

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
tf: Normal melting (fusion) point

Latest version available from:

<https://www.chemeo.com/cid/123-653-0/2-4-Pregnadien-2-3-d-isoxazol-17-alpha-ethynyl-17-beta-ol-TMS.pdf>

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