2,4-Pregnadien-(2,3-d)isoxazol-17.alpha.-ethynyl-1
TMS

InChI: 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
InchiKey: 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