MLS003115428

Other names: danazol
Inchi: InChI=1S/C22H27NO2/c1-4-22(24)10-8-18-16-6-5-15-11-19-14(13-23-25-19)12-20(15,2)
InchiKey: POZRVZJJTULAOH-UHFFFAOYSA-N
Formula: C22H27NO2
SMILES: C#CC1(O)CCC2C3CCC4=Cc5oncc5CC4(C)C3CCC21C
Mol. weight [g/mol]: 337.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.51		Aqueous Solubility Prediction Method
log10ws	-5.51		Estimated Solubility Method
log10ws	-5.51		Aqueous and cosolvent solubility data for drug-like organic compounds
logp	4.221		Crippen Method
mcvol	266.760	ml/mol	McGowan Method
tf	498.75	K	Aqueous Solubility Prediction Method

Sources

Aqueous and cosolvent solubility data for drug-like organic compounds: https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient

mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point