N-ALLYLNORMETAZOCINE

Other names: 2'-Hydroxy-5,9-dimehtyl-2-allyl-6,7-benzomorphan
SKF-10,047
WIN 19631
Inchi: InChI=1S/C17H23NO/c1-4-8-18-9-7-17(3)12(2)16(18)10-13-5-6-14(19)11-15(13)17/h4-6,
InchiKey: LGQCVMYAEFTEFN-UHFFFAOYSA-N
Formula: C17H23NO
SMILES: C=CCN1CCC2(C)c3cc(O)ccc3CC1C2C
Mol. weight [g/mol]: 257.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Cheméo Relay (1.0)
logp	3.102		Crippen Method
mcvol	216.460	ml/mol	McGowan Method
tf	414.05	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7619354&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point