

2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-3-allyl-6,11-dimethyl-

Other names:

SKF-10,047

WIN 19631

2'-Hydroxy-5,9-dimethyl-2-allyl-6,7-benzomorphan

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]:

257.37

CAS:

7619-35-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.31		Crippen Method
logp	3.102		Crippen Method
mcvol	216.460	ml/mol	McGowan Method

Sources

Crippen Method:

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

Crippen Method:

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

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C7619354&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

Latest version available from:

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