Cyclazocine

Other names:	2,6-Methano-3-benzazocin-8-ol, 3-(cyclopropylmethyl)-1,2,3,4,5,6-hexahydro-6,11-dimethyl-
	NIH 7981
	UM 407
	Win 20740
	WIN 20,740
	2-Cyclopropylmethyl-2'-hydroxy-5,9-dimethyl-6,7-benzomorphan
	2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-3-(cyclopropylmethyl)-6,11-dimethyl-
	3-(Cyclopropylmethyl)-1,2,3,4,5,6-hexahydro-6,11-dimethyl-2,6-methano-3-benzazocin-8-
	3-Cyclopropylmethyl-6(eq),11(ax)-dimethyl-2,6-methano-3-benzazocin-8-ol
	2-Cyclopropylmethyl-5,9-dimethyl-2'-hydroxy-6,7-benzomorphan
	NSC-107429
Inchi:	InChI=1S/C18H25NO/c1-12-17-9-14-5-6-15(20)10-16(14)18(12,2)7-8-19(17)11-13-3-4-13
InchiKey:	YQYVFVRQLZMJKJ-UHFFFAOYSA-N
Formula:	C18H25NO
SMILES:	CC1C2Cc3ccc(O)cc3C1(C)CCN2CC1CC1
Mol. weight [g/mol]:	271.40
CAS:	3572-80-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	3.326		Crippen Method
mcvol	223.990	ml/mol	McGowan Method

Sources

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=C3572803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume