

CYCLAZOCINE

Other names:	2,6-Methano-3-benzazocin-8-ol, 3-(cyclopropylmethyl)-1,2,3,4,5,6-hexahydro-6,11-dimethyl- NIF 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-ol 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)11-13-3-4-1
InchiKey:	YQYVFVRQLZMJJKJ-UHFFFAOYSA-N
Formula:	C18H25NO
SMILES:	CC1C2Cc3ccc(O)cc3C1(C)CCN2CC1CC1
Mol. weight [g/mol]:	271.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Cheméo Relay (1.0)
logp	3.326		Crippen Method
mcvol	223.990	ml/mol	McGowan Method
tf	441.11	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3572803&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
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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