Pentazocine

Other names:	(.+/-.)-Pentazocine
	(2R*,6R*,11R*)-1,2,3,4,5,6-Hexahydro-6,11-dimethyl-3-(3-methyl-2-butenyl)-2,6-methanc
	1,2,3,4,5,6-Hexahydro-6,11-dimethyl-3-(3-methyl-2-butenyl)-2,6-methano-3-benzazocin-8
	2'-Hydroxy-5,9-dimethyl-2-(3,3-dimethylallyl)-6,7-benzomorphan
	2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-(3-methyl-2-butenyl)-
	2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-(3-methyl-2-butenyl)-, (2R,6R,11R)-rel-
	2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-(3-methyl-2-butenyl)-, (2«alpha»,6«alpha»,11R)-
	2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-(3-methyl-2-butenyl)-, (2«alpha»,6«alpha»,11R*)-
	2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-(3-methyl-2-butenyl)-, (2A«alphaA»,6A«alphaA»,11R)-
	2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-(3-methyl-2-butenyl)-, (2A«alphaA»,6A«alphaA»,11R*)-
	2-(3,3-Dimethylallyl)-2'-hydroxy-5,9-dimethyl-6,7-benzomorphan
	2-(3,3-Dimethylallyl)cyclazocine
	2-Dimethylallyl-5,9-dimethyl-2'-hydroxybenzomorphan
	3-(3-Methyl-2-butenyl)-1,2,3,4,5,6-hexahydro-6,11-dimethyl-2,6-methano-3-benzazocin-8
	Fortalgesic
	Fortalin
	Fortral
	II-C-2
	KF-1820
	L-pentazocine
	Liticon
	NIH 7958
	NSC-107430
	Pentagin
	Pentazocaine
	Pentazocin
	Sosegon
	Soseton
	Sosigon
	Talwan
	Talwin
	Win 20228
	dl-2'-Hydroxy-5,9-dimethyl-2-(3,3-dimethylallyl)-6,7-benzomorphan
	dl-pentazocine
Inchi:	InChI=1S/C19H27NO/c1-13(2)7-9-20-10-8-19(4)14(3)18(20)11-15-5-6-16(21)12-17(15)19
InchiKey:	VOKSWYLNZZRQPF-UHFFFAOYSA-N
Formula:	C19H27NO
SMILES:	CC(C)=CCN1CCC2(C)c3cc(O)ccc3CC1C2C
Mol. weight [g/mol]:	285.42
CAS:	359-83-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Aqueous Solubility Prediction Method
logp	3.883		Crippen Method
mcvol	244.640	ml/mol	McGowan Method
rinpol	2286.00		NIST Webbook
rinpol	2246.00		NIST Webbook
rinpol	2285.00		NIST Webbook
rinpol	2262.00		NIST Webbook
rinpol	2246.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2286.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2262.00		NIST Webbook
rinpol	2265.00		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2262.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2280.00		NIST Webbook
tf	419.30	K	Aqueous Solubility Prediction Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C359831&Units=SI

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

Legend

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