Phenazocine

Other names: 2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-(2-phenylethyl)-
2,6-Methano-3-benzazocin-8-ol, 1,2,3,4,5,6-hexahydro-6,11-dimethyl-3-phenethyl-
NIH 7519
Prinadol
SKF 6574
6,11-Dimethyl-1,2,3,4,5,6-hexahydro-8-hydroxy-3-phenethyl-2,6-methano-3-benzazocine
1,2,3,4,5,6-Hexahydro-6,11-dimethyl-3-phenethyl-2,6-methano-3-benzazocin-8-ol
1,2,3,4,5,6-Hexahydro-8-hydroxy-6,11-dimethyl-3-phenethyl-2,6-methano-3-benzazocine
2'-Hydroxy-5,9-dimethyl-2-phenethyl-6,7-benzomorphan
1,2,3,4,5,6-Hexahydro-6,11-dimethyl-3-(2-phenylethyl)-2,6-methano-3-benzazocin-8-ol
Phenethylazocine
Phenobenzorphan

Inchi: InChI=1S/C22H27NO/c1-16-21-14-18-8-9-19(24)15-20(18)22(16,2)11-13-23(21)12-10-17

InchiKey: ZQHYKVKNPWDQSL-UHFFFAOYSA-N

Formula: C22H27NO

SMILES: CC1C2Cc3ccc(O)cc3C1(C)CCN2CCc1ccccc1

Mol. weight [g/mol]: 321.46

CAS: 127-35-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	4.159		Crippen Method
mcvol	267.450	ml/mol	McGowan Method
rinpol	2677.00		NIST Webbook
rinpol	2720.00		NIST Webbook
rinpol	2684.00		NIST Webbook
rinpol	2677.00		NIST Webbook

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=C127355&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
rinpol:	Non-polar retention indices