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

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Cheméo Relay (1.0)
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
tf	446.76	K	Cheméo Relay (1.0)

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C127355&Units=SI

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