

Phenomorphan

Other names:	Morphinan-3-ol, 17-(2-phenylethyl)- Morphinan-3-ol, 17-phenethyl-, (-)- 3-Hydroxy-N-phenethylmorphinan NIH-7274
Inchi:	InChI=1S/C24H29NO/c26-20-10-9-19-16-23-21-8-4-5-12-24(21,22(19)17-20)13-15-25(23)
InchiKey:	CFBQYWXPZVQQTN-UHFFFAOYSA-N
Formula:	C24H29NO
SMILES:	<chem>Oc1ccc2c(c1)C13CCCCC1C(C2)N(CCCc1ccccc1)CC3</chem>
Mol. weight [g/mol]:	347.49
CAS:	468-07-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.39		Crippen Method
logp	4.693		Crippen Method
mcvol	284.770	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C468075&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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