Neopine

Other names:	Morphinan-6-ol, 8,14-didehydro-4,5-epoxy-3-methoxy-17-methyl-, (5«alpha»,6«alpha»)- Morphinan-6«alpha»-ol, 8,14-didehydro-4,5«alpha»-epoxy-3-methoxy-17-methyl-«beta»-Codeine Neopin 8,14-Didehydro-4,5«alpha»-epoxy-3-methoxy-17-methylmorphinan-6«alpha»-ol (5«alpha»,6«alpha»)-8,14-didehydro-4,5-epoxy-3-methoxy-17-methylmorphinan-6-ol
Inchi:	InChI=1S/C18H21NO3/c1-19-8-7-18-11-4-5-13(20)17(18)22-16-14(21-2)6-3-10(15(16)18
InchiKey:	NNDKZTBFZTWKLA-UHFFFAOYSA-N
Formula:	C18H21NO3
SMILES:	COc1ccc2c3c1OC1C(O)CC=C4C(C2)N(C)CCC431
Mol. weight [g/mol]:	299.36
CAS:	467-14-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.10		Crippen Method
logp	1.645		Crippen Method
mcvol	220.570	ml/mol	McGowan Method
rinpol	2395.00		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=C467141&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