Desomorphine

Other names:	Morphinan-3-ol, 4,5-epoxy-17-methyl-, (5«alpha»)-
	Morphine, 6-deoxy-7,8-dihydro-
	Deoxydihydromorphine D
	Dihydrodeoxymorphine
	Dihydrodesoxymorphine
	Morphine D, deoxydihydro-
	Permonid
	4,5-Epoxy-3-hydroxy-N-methylmorphinan
	Morphinan-3-ol, 4,5-«alpha»-epoxy-17-methyl-
	Desomorfin
	Dihydrodesoxymorphine-D
	Dihydroepoxymorphine
	Desmorphine
	6-Deoxy-7,8-dihydromorphine
Inchi:	InChI=1S/C17H21NO2/c1-18-8-7-17-11-3-2-4-14(17)20-16-13(19)6-5-10(15(16)17)9-12(
InchiKey:	LNNWVNGFPYWNQE-UHFFFAOYSA-N
Formula:	C17H21NO2
SMILES:	CN1CCC23c4c5ccc(O)c4OC2CCCC3C1C5
Mol. weight [g/mol]:	271.35
CAS:	427-00-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	2.451		Crippen Method
mcvol	204.910	ml/mol	McGowan Method
rinpol	2295.00		NIST Webbook
rinpol	2232.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C427009&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices