Morphinan-3-ol, 4,5-epoxy-17-methyl-, (5.alpha.)-

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]: 271.36

Physical Properties

Property code	Value	Unit	Source
ie	7.60	eV	Cheméo Relay (1.0)
log10ws	-2.25		Cheméo Relay (1.0)
logp	2.451		Crippen Method
mcvol	204.910	ml/mol	McGowan Method
rinpol	2295.00		NIST Webbook
rinpol	2232.00		NIST Webbook
tf	406.46	K	Cheméo Relay (1.0)

Sources

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=C427009&Units=SI

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
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