Dihydromorphine

Other names:	Morphinan-3,6-diol, 4,5-epoxy-17-methyl-, (5«alpha»,6«alpha»)- Hydromorphine Paramorfan Paramorphan Morphinan-3,6«alpha»-diol, 4,5«alpha»-epoxy-17-methyl- Morphine, dihydro- Dihydromorfin 6«alpha»-Hydromorphol «alpha»-Dihydromorphine Morphine, 7,8-dihydro- (5«alpha»,6«alpha»)-4,5-Epoxy-17-methylmorphinan-3,6-diol 7,8-Dihydromorphine NSC 117865 4,5-Epoxy-3-hydroxy-17-methylmorphinan-6-one (hydromorphone)
Inchi:	InChI=1S/C17H21NO3/c1-18-7-6-17-10-3-5-13(20)16(17)21-15-12(19)4-2-9(14(15)17)8-
InchiKey:	IJVCSMSMFSCRME-UHFFFAOYSA-N
Formula:	C17H21NO3
SMILES:	CN1CCC23c4c5ccc(O)c4OC2C(O)CCC3C1C5
Mol. weight [g/mol]:	287.35
CAS:	509-60-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	1.422		Crippen Method
mcvol	210.780	ml/mol	McGowan Method
rinpol	2450.00		NIST Webbook
rinpol	2451.00		NIST Webbook
rinpol	2467.00		NIST Webbook
rinpol	2451.00		NIST Webbook
rinpol	2534.60		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	35.61	kJ/mol	539.20	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C509604&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices