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]:	287.36

Physical Properties

Property code	Value	Unit	Source
ie	7.87	eV	Cheméo Relay (1.0)
log10ws	-1.52		Cheméo Relay (1.0)
logp	1.422		Crippen Method
mcvol	210.780	ml/mol	McGowan Method
rinpol	2534.60		NIST Webbook
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
tf	424.51	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

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

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

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=C509604&Units=SI

Legend

hfust: Enthalpy of fusion at a given temperature

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