morphine

Other names:	(-)-Morphine
	(5«alpha»,6«alpha»)-7,8-Didehydro-4,5-epoxy-17-methylmorphinan-3,6-diol
	9H-9,9c-Iminoethanophenanthro(4,5-bcd)furan-3,5-diol, 4a,5,7a,8-tetrahydro-12-methyl-
	Avinza
	DepoDur
	Dulcontin
	Duromorph
	Kadain
	M-Eslon
	MS contin
	Meconium
	Morfina
	Morphia
	Morphin
	Morphina
	Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-methyl- (5.alpha.,6.alpha.)-
	Morphinan-3,6-diol, 7,8-didehydro-4,5-epoxy-17-methyl- (5«alpha»,6«alpha»)-
	Morphinan-3,6«alpha»-diol, 7,8-didehydro-4,5«alpha»-epoxy-17-methyl-
	Morphinism
	Morphinum
	Morphium
	Nepenthe
	Oramorph SR
	Ospalivina
	Roxanol
	Statex SR
	l-Morphine
Inchi:	InChI=1S/C17H19NO3/c1-18-7-6-17-10-3-5-13(20)16(17)21-15-12(19)4-2-9(14(15)17)8-
InchiKey:	BQJCRHHNABKAKU-UHFFFAOYSA-N
Formula:	C17H21NO4
SMILES:	CN1CCC23c4c5ccc(O)c4OC2C(O)C=CC3C1C5
Mol. weight [g/mol]:	303.35

Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	Cheméo Relay (1.0)

log10ws	-3.18		Aqueous Solubility Prediction Method
logp	1.198		Crippen Method
mcvol	206.480	ml/mol	McGowan Method
tf	437.99	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B8001639&Units=SI&Mask=3FFF

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

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

Cheméo Relay (1.0):

Legend

ie: Ionization energy

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

tf: Normal melting (fusion) point