Ethylmorphine

Other names:	3-Ethoxymorphine
	3-O-Ethylmorphine
	Codethyline
	Dionin
	Dionine
	Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-ethoxy-17-methyl-, (5.alpha.,6.alpha.)-
	Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-ethoxy-17-methyl-, (5«alpha»,6«alpha»)-
	Morphinan-6-ol, 7,8-didehydro-4,5-epoxy-3-ethoxy-17-methyl-, (5Â«alphaÂ»,6Â«alphaÂ»)-
	Morphinan-6«alpha»-ol, 7,8-didehydro-4,5«alpha»-epoxy-3-ethoxy-17-methyl-
	Morphinan-6Â«alphaÂ»-ol, 7,8-didehydro-4,5Â«alphaÂ»-epoxy-3-ethoxy-17-methyl-
	Morphine, 3-O-ethyl-
	Morphine, ethyl-
Inchi:	InChI=1S/C19H23NO3/c1-3-22-15-7-4-11-10-13-12-5-6-14(21)18-19(12,8-9-20(13)2)16(1
InchiKey:	OGDVEMNWJVYAJL-UHFFFAOYSA-N
Formula:	C19H23NO3
SMILES:	CCOc1ccc2c3c1OC1C(O)C=CC4C(C2)N(C)CCC341
Mol. weight [g/mol]:	313.39
CAS:	76-58-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.82		Aqueous Solubility Prediction Method
logp	1.891		Crippen Method
mcvol	234.660	ml/mol	McGowan Method
rinpol	2405.00		NIST Webbook
rinpol	2400.00		NIST Webbook
rinpol	2415.00		NIST Webbook
rinpol	2415.00		NIST Webbook
rinpol	2411.00		NIST Webbook
rinpol	2405.00		NIST Webbook
rinpol	2411.00		NIST Webbook
rinpol	2415.00		NIST Webbook
rinpol	2390.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C76584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Legend

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