Etorphine

Other names:	6,14-Ethenomorphinan-7-methanol, 4,5-epoxy-3-hydroxy-6-methoxy-«alpha»,17-dimethyl-«alpha»-propyl-, [5«alpha»,7«alpha»(R)]-
	6,14-endo-Ethenotetrahydrooripavine, 7«alpha»-(1-hydroxy-1-methylbutyl)-7«alpha»-Etorphine
	7,8-Dihydro-7-«alpha»-(1-(R)-hydroxy-1-methylbutyl)-O
Inchi:	InChI=1S/C25H33NO4/c1-5-8-22(2,28)17-14-23-9-10-25(17,29-4)21-24(23)11-12-26(3)1
InchiKey:	CAHCBJPUTCKATP-UHFFFAOYSA-N
Formula:	C25H33NO4
SMILES:	CCCC(C)(O)C1CC23C=CC1(OC)C1Oc4c(O)ccc5c4C12CCN(C)C3C5
Mol. weight [g/mol]:	411.53
CAS:	14521-96-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.49		Crippen Method
logp	3.164		Crippen Method
mcvol	314.210	ml/mol	McGowan Method
rinpol	3033.00		NIST Webbook
rinpol	3033.00		NIST Webbook
rinpol	3033.00		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=C14521961&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices