Etomidate

Other names:	(+)-Ethyl 1-(«alpha»-methylbenzyl)imidazole-5-carboxylate
	(+)-Ethyl 1-(Â«alphaÂ»-methylbenzyl)imidazole-5-carboxylate
	(+)-Etomidate
	(R)-(+)-1-(«alpha»-Methylbenzyl)imidazole-5-carboxylic acid ethyl ester
	(R)-(+)-1-(Â«alphaÂ»-Methylbenzyl)imidazole-5-carboxylic acid ethyl ester
	1-(1-Phenylethyl)-1H-imidazole-5-carboxylic acid ethyl ester
	1-(«alpha»-Methylbenzyl)-1H-imidazole-5-carboxylic acid ethyl ester
	1-(Â«alphaÂ»-Methylbenzyl)-1H-imidazole-5-carboxylic acid ethyl ester
	1H-Imidazole-5-carboxylic acid, 1-(1-phenylethyl)-, ethyl ester, (+)-
	1H-Imidazole-5-carboxylic acid, 1-(1-phenylethyl)-, ethyl ester, (R)-
	1H-Imidazole-5-carboxylic acid, 1-(«alpha»-methylbenzyl)-, ethyl ester, (+)-
	1H-Imidazole-5-carboxylic acid, 1-(Â«alphaÂ»-methylbenzyl)-, ethyl ester, (+)-
	Amidate
	Amidate (pharmaceutical)
	Ethyl 1-(1-phenylethyl)-1H-imidazole-5-carboxylate, (+)-
	Hypnomidate
	Imidazole-5-carboxylic acid, 1-(«alpha»-methylbenzyl)-, ethyl ester, (R)-(+)-
	Imidazole-5-carboxylic acid, 1-(Â«alphaÂ»-methylbenzyl)-, ethyl ester, (R)-(+)-
	R 16659
	R-(+)-Ethyl 1-(1-phenylethyl)-1H-imidazole-5-carboxylate
	Radenarcon
	d-Etomidate
Inchi:	InChI=1S/C14H16N2O2/c1-3-18-14(17)13-9-15-10-16(13)11(2)12-7-5-4-6-8-12/h4-11H,3
InchiKey:	NPUKDXXFDDZOKR-UHFFFAOYSA-N
Formula:	C14H16N2O2
SMILES:	CCOC(=O)c1cncn1C(C)c1ccccc1
Mol. weight [g/mol]:	244.29
CAS:	33125-97-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Aqueous Solubility Prediction Method
log10ws	-4.74		Estimated Solubility Method
log10ws	-6.74		Aqueous and cosolvent solubility data for drug-like organic compounds

logp	2.669		Crippen Method
mcvol	192.300	ml/mol	McGowan Method
rinpol	2008.00		NIST Webbook

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Aqueous and cosolvent solubility data for drug-like organic compounds:	https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2751500/
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C33125972&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