ETOMIDATE

Other names: (+)-Ethyl 1-(«alpha»-methylbenzyl)imidazole-5-carboxylate
(+)-Etomidate
(R)-(+)-1-(«alpha»-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
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, (+)-
Amidate
Amidate (pharmaceutical)
Ethyl 1-(1-phenylethyl)-1H-imidazole-5-carboxylate, (+)-
Hypnomidate
Imidazole-5-carboxylic acid, 1-(«alpha»-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

Physical Properties

Property code	Value	Unit	Source
af	0.6201		Cheméo Relay (1.0)
hf	-178.99	kJ/mol	Cheméo Relay (1.0)
hvap	90.75	kJ/mol	Cheméo Relay (1.0)
ie	8.36	eV	Cheméo Relay (1.0)
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

pc	2244.04	kPa	Cheméo Relay (1.0, beta)
rinpol	2008.00		NIST Webbook
tb	612.97	K	Cheméo Relay (1.0)
tc	867.01	K	Cheméo Relay (1.0)
tf	307.19	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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/

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33125972&Units=SI

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

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

Legend

af: Acentric Factor
hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point