Carbimazole

Other names:	1H-Imidazole-1-carboxylic acid, 2,3-dihydro-3-methyl-2-thioxo-, ethyl ester
	Ethyl 3-methyl-2-thioimidazoline-1-carboxylate
	4-Imidazoline-1-carboxylic acid, 3-methyl-2-thioxo-, ethyl ester
	Athyromazole
	Basolest
	Carbethoxymethimazole
	Carbimazol
	Carbinazole
	CG1
	3-Methyl-2-thioxo-4-imidazoline-1-carboxylic acid ethyl ester
	Neomercazole
	Tyrazol
	Neo-thyreostat
Inchi:	InChI=1S/C7H10N2O2S/c1-3-11-7(10)9-5-4-8(2)6(9)12/h4-5H,3H2,1-2H3
InchiKey:	CFOYWRHIYXMDOT-UHFFFAOYSA-N
Formula:	C7H10N2O2S
SMILES:	CCOC(=O)n1ccn(C)c1=S
Mol. weight [g/mol]:	186.23
CAS:	22232-54-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	1.561		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
rinpol	1678.00		NIST Webbook

Sources

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=C22232548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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