Ornidazole

Other names:	1H-Imidazole-1-ethanol, «alpha»-(chloromethyl)-2-methyl-5-nitro-
	«alpha»-(Chloromethyl)-2-methyl-5-nitroimidazole-1-ethanol
	Imidazole-1-ethanol, «alpha»-(chloromethyl)-2-methyl-5-nitro-
	Madelen
	Ro 7-0207
	Tiberal
	1-(2-Hydroxy-3-chloropropyl)-2-methyl-5-nitroimidazole
	1-(3-Chloro-2-hydroxypropyl)-2-methyl-5-nitroimidazole
	«alpha»-(Chlormethyl)-2-methyl-5-nitro-imidazol-1-aethanol
	«alpha»-(Chloromethyl)-2-methyl-5-nitro-1H-imidazole-1-ethanol
	Ornidal
	(.+/-.)-Ornidazole
	NSC 95075
	1-(2-Hydroxy-3-chloropropyl)-2-methyl-5-nitroimidazole (ornidazole)
Inchi:	InChI=1S/C7H10ClN3O3/c1-5-9-3-7(11(13)14)10(5)4-6(12)2-8/h3,6,12H,2,4H2,1H3
InchiKey:	IPWKIXLWTCNBKN-UHFFFAOYSA-N
Formula:	C7H10ClN3O3
SMILES:	Cc1ncc([N+](=O)[O-])n1CC(O)CCl
Mol. weight [g/mol]:	219.63
CAS:	16773-42-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Crippen Method
logp	0.699		Crippen Method
mcvol	145.520	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	21.38	kJ/mol	358.60	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16773425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hfust:	Enthalpy of fusion at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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