

Metronidazole

Other names:

1-(2-Hydroxy-1-ethyl)-2-methyl-5-nitroimidazole
1-(2-hydroxyethyl)-2-methyl-5-nitroimidazole
1-(«beta»-Ethylol)-2-methyl-5-nitro-3-azapyrrole
1-(«beta»-Hydroxyethyl)-2-methyl-5-nitroimidazole
1-(«beta»-Oxyethyl)-2-methyl-5-nitroimidazole
1-(«beta»-Ethylol)-2-methyl-5-nitro-3-azapyrrole
1-(«beta»-Hydroxyethyl)-2-methyl-5-nitroimidazole
1-(«beta»-Oxyethyl)-2-methyl-5-nitroimidazole
1-Hydroxyethyl-2-methyl-5-nitroimidazole
1H-Imidazole-1-ethanol, 2-methyl-5-nitro-
2-(2-Methyl-5-nitro-1H-imidazol-1-yl)ethanol
2-Methyl-1-(2-hydroxyethyl)-5-nitroimidazole
2-Methyl-3-(2-hydroxyethyl)-4-nitroimidazole
2-Methyl-5-nitroimidazole-1-ethanol
2-methyl-5-nitro-1H-imidazole-1-ethanol
Acromona
Anagiardil
Arilin
Atrivyl
Bayer 5360
Bexon
Cimetrol 500LPCI
Clont
Cont
Danizol
Deflamon
Deflamon-Wirkstoff
Efloran
Elyzol
Entizol
Eumin
Flagemona
Flagesol
Flagil
Flagyl
Flazol
Flegyl
Fossyol
Giatricol
Gineflavir

Imidazole-1-ethanol, 2-methyl-5-nitro-
Klion
Klont
Meronidal
Methronidazole
Metro I.V.
Metro cream & gel
MetroGel
Metrolag
Metrolyl
Metron
Metronidaz
Metronidazol
Metronidazole - from non-authenticated sample -
Metronidazole Benzoate
Metronidazolo
Metrotop
Mexibol
Monagyl
Monasin
NSC-50364
Nalox
Nida
Novonidazol
Orvagil
Polibiotic
Protostat
RP 8823
Rathimed
SC 10295
Sanatrichom
Satric
Takimetol
Trichazol
Trichex
Tricho cordes
Tricho-gynaedron
Trichobrol
Trichocide
Trichomol
Trichomonacid 'pharmachim'
Trichopal
Trichopol

Tricocet
 Tricom
 Tricowas B
 Trikacide
 Trikamon
 Trikhopol
 Trikojol
 Trikozol
 Trimeks
 Trivazol
 Vagilen
 Vagimid
 Vertisal
 Wagitran
 Zadstat
 component of Flagyl i.v.
 component of Metro i.v.
 component of Rtu
 neo-Tric

Inchi: InChI=1S/C6H9N3O3/c1-5-7-4-6(9(11)12)8(5)2-3-10/h4,10H,2-3H2,1H3
InchiKey: VAOCPAMSLUNLGC-UHFFFAOYSA-N
Formula: C6H9N3O3
SMILES: Cc1ncc([N+](=O)[O-])n1CCO
Mol. weight [g/mol]: 171.15
CAS: 443-48-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.52		Aqueous Solubility Prediction Method
log10ws	-1.22		Estimated Solubility Method
logp	0.092		Crippen Method
mcvol	119.190	ml/mol	McGowan Method
rinpol	1618.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1592.00		NIST Webbook

Sources

Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C443481&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Investigation on molecular interactions of antibiotics in alcohols using aqueous solubility predictions at different temperatures:	https://www.doi.org/10.1016/j.jct.2016.09.037
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

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