

Minoxidil

Other names:

2,3-Dihydro-3-hydroxy-2-imino-6-(1-piperidiny)-4-pyrimidinamine
2,4-Diamino-6-piperidinilpirimidina-3-ossido
2,4-Diamino-6-piperidinopyrimidine 3-N-oxide
2,4-Diamino-6-piperidinopyrimidine 3-oxide
2,4-Pyrimidinediamine, 6-(1-piperidiny)-, 3-oxide
6-(1-Piperidiny)-2,4-pyrimidinediamine 3-oxide
6-Amino-1,2-dihydro-1-hydroxy-2-imino-4-piperidinopyrimidine
6-Piperidino-2,4-diaminopyrimidine 3-oxide
Alopexil
Alostil
Loniten
Lonolox
Minossidile
Minoximen
Normoxidil
PDP
Pierminox
Prexidil
Pyrimidine, 2,4-diamino-6-piperidino-, 3-oxide
Regaine
Rogaine
Tricoxidil
Trocoxidil
U 10858
U-10,858

Inchi:

InChI=1S/C9H15N5O/c10-7-6-8(12-9(11)14(7)15)13-4-2-1-3-5-13/h6H,1-5,10H2,(H2,11,

InchiKey:

ZFMITUMMTDLWHR-UHFFFAOYSA-N

Formula:

C9H15N5O

SMILES:

Nc1cc(N2CCCCC2)nc(N)[n+][O-]

Mol. weight [g/mol]:

209.25

CAS:

38304-91-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.91		Aqueous Solubility Prediction Method

log10ws	-1.99		Estimated Solubility Method
logp	-0.130		Crippen Method
mcvol	158.820	ml/mol	McGowan Method

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=C38304915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Solubility of Minoxidil in Methanol, Ethanol, 1-Propanol, 2-Propanol, Acetone, and Water (at 25°C):	https://www.doi.org/10.1021/je1012839
Aqueous Solubility Prediction Method: 333.15) K:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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