

Ethirimol

Other names:

2-Ethylamino-4-methyl-5-n-butyl-6-hydroxypyrimidine
4(1H)-Pyrimidinone, 5-butyl-2-(ethylamino)-6-methyl-
4(3H)-Pyrimidinone, 5-butyl-2-(ethylamino)-6-methyl-
5-Butyl-2-(ethylamino)-4-hydroxy-6-methylpyrimidine
5-Butyl-2-(ethylamino)-6-methyl-4(1H)-pyrimidinone
5-Butyl-2-ethylamino-6-methylpyrimidin-4-ol
5-n-Butyl-2-ethylamino-4-hydroxy-6-methylpyrimidine
Ethirimal
Ethrimiol
Ethyrimol
Milgo
Milgo E
Milstem
Milstem seed dressing
NSC 263491
New milstem
PP 149

Inchi:

InChI=1S/C11H19N3O/c1-4-6-7-9-8(3)13-11(12-5-2)14-10(9)15/h4-7H2,1-3H3,(H2,12,13)

InchiKey:

BBXXLROWFHWY-UHFFFAOYSA-N

Formula:

C11H19N3O

SMILES:

CCCCc1c(C)[nH]c(NCC)nc1=O

Mol. weight [g/mol]:

209.29

CAS:

23947-60-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.02		Aqueous Solubility Prediction Method
log10ws	-3.03		Estimated Solubility Method
logp	1.371		Crippen Method
mccvol	177.900	ml/mol	McGowan Method
tf	434.35 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	20.32	kJ/mol	432.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23947606&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
tf:	Normal melting (fusion) point

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