2,4-Pyrimidinediamine, 5-(4-chlorophenyl)-6-ethyl-

Other names: 2,4-Diamino-5-(4-chlorophenyl)-6-ethylpyrimidine
2,4-Diamino-5-(p-chlorophenyl)-6-ethylpyrimidine
2,4-Diamino-5-chlorophenyl-6-ethylpyrimidine
2,4-Pyrimidinediamine, 5-(p-chlorophenyl)-6-ethyl-
4753 R.P.
5-(4'-Chlorophenyl)-2,4-diamino-6-ethylpyrimidine
5-(4-Chlorophenyl)-6-ethyl-2,4-pyrimidinediamine
BW 50-63
Chloridin
Chloridine
Chloridyn
Darachlor
Darapram
Daraprim
Daraprime
Diaminopyritamin
Erbaprelina
Khloridin
Malacid
Malocid
Malocide
Maloprim
NCI-C01683
NSC-3061
Pirimecidan
Pirimetamin
Pirimetamina
Primethamine
Pyrimethamin
Pyrimidine, 2,4-diamino-5-(p-chlorophenyl)-6-ethyl-
RP 4753
Tindurin
Tinduring
WR 2978
pyrimethamine

Inchi: InChI=1S/C12H13ClN4/c1-2-9-10(11(14)17-12(15)16-9)7-3-5-8(13)6-4-7/h3-6H,2H2,1H3

InchiKey: WKSAUQYGYAYLPV-UHFFFAOYSA-N

Formula: C12H13ClN4

SMILES: CCc1nc(N)nc(N)c1-c1ccc(Cl)cc1

Mol. weight [g/mol]: 248.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.11		Aqueous Solubility Prediction Method
logp	2.524		Crippen Method
mcvol	184.580	ml/mol	McGowan Method
rinpol	2140.00		NIST Webbook
rinpol	2138.00		NIST Webbook
rinpol	2140.00		NIST Webbook
tf	506.48	K	Aqueous Solubility Prediction Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58140&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

tf: Normal melting (fusion) point