

Triamterene

Other names:

2,4,7-Pteridinetriamine, 6-phenyl-
2,4,7-Triamino-6-fenilpteridina
2,4,7-Triamino-6-phenylpteridine
6-Phenyl-2,4,7-pteridinetriamine
6-Phenyl-2,4,7-triaminopteridine
Ademin
Ademine
Diren
Ditak
Diurene
Dyren
Dyrenium
Dytac
Jatropur
NCI-C56042
NSC-77625
Noridil
Noridyl
Pteridine, 2,4,7-triamino-6-phenyl-
Pterofen
Pterophene
SK&F 8542
SKF 8542
Taturil
Teriam
Teridin
Tri-span
Triampur
Triamteren
Triamteril
Triamteril complex
Triteren
Urocaudal

Inchi:

InChI=1S/C12H11N7/c13-9-7(6-4-2-1-3-5-6)16-8-10(14)18-12(15)19-11(8)17-9/h1-5H,(H

InchiKey:

FNYLWPVRPXGIIP-UHFFFAOYSA-N

Formula:

C12H11N7

SMILES:

Nc1nc(N)c2nc(-c3ccccc3)c(N)nc2n1

Mol. weight [g/mol]:

253.26

CAS:

396-01-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Aqueous Solubility Prediction Method
log10ws	-2.40		Estimated Solubility Method
logp	0.833		Crippen Method
mcvol	182.820	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C396010&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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