2,4,7-Pteridinetriamine, 6-phenyl-

Other names:	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
	triamterene
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]:	253.27

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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

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