2,6-Pyridinediamine, 3-(phenylazo)-

Other names:	2,6-Diamino-3-(phenylazo)pyridine
	3-(Phenylazo)-2,6-pyridinediamine
	3-[(E)-Phenyldiazenyl]-2,6-pyridinediamine
	AP
	DPP
	Diridone
	Gastracid
	Gastrotest
	Mallophene
	NC 150
	NSC 145895
	Phenazodine
	Phenazopryidine
	Phenazopyridine
	Phenylazo tablet
	Pirid
	Plegomazin
	Proma
	Promactil
	Promazil
	Prozil
	Pyrazofen
	Pyridacil
	Pyridine, 2,6-diamino-3-(phenylazo)-
	Pyridium
	Pyripyridium
	Sanopron
	Sedural
	Uridinal
	Urodine
	W 1655
	oxytetracycline
Inchi:	InChI=1S/C11H11N5/c12-10-7-6-9(11(13)14-10)16-15-8-4-2-1-3-5-8/h1-7H,(H4,12,13,14
InchiKey:	QPFYXYFORQJZEC-UHFFFAOYSA-N
Formula:	C11H11N5
SMILES:	Nc1ccc(N=Nc2ccccc2)c(N)n1
Mol. weight [g/mol]:	213.24
CAS:	94-78-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.09		Aqueous Solubility Prediction Method
logp	2.661		Crippen Method
mcvol	163.930	ml/mol	McGowan Method
rinpol	2345.00		NIST Webbook
rinpol	2346.00		NIST Webbook
rinpol	2345.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2280.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2345.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C94780&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices