Tripelennamine

Other names:	1,2-Ethanediamine, N,N-dimethyl-N'-(phenylmethyl)-N'-2-pyridinyl-
	2-(N-Benzyl-N-(2-dimethylaminoethyl)amino)pyridine
	2-[Benzyl(2-Dimethylaminoethyl)amino]pyridine
	2750 R.P.
	Benzoxale
	Benzyl-«alpha»-pyridyl-dimethyl-aethylendiamin
	Benzyl-Â«alphaÂ»-pyridyl-dimethyl-aethylendiamin
	Cizaron
	Ethylenediamine, N-benzyl-N',N'-dimethyl-N-(2-pyridyl)-
	N,N-Dimethyl-N'-benzyl-N'-(2-pyridyl)ethylenediamine
	N,N-Dimethyl-N'-benzyl-N'-(«alpha»-pyridyl)ethylenediamine
	N,N-Dimethyl-N'-benzyl-N'-(Â«alphaÂ»-pyridyl)ethylenediamine
	N-Benzyl-N',N'-dimethyl-N-(2-pyridyl)ethylenediamine
	N-Benzyl-N-(2-pyridyl)-N',N'-dimethyl ethylenediamine
	NCI-C60662
	NSC 118946
	PBZ
	Piribenzil
	Pyribenzamin
	Pyribenzamine
	Pyridbenzamine
	Pyridine, 2-[benzyl[2-(dimethylamino)ethyl]amino]-
	Pyrinamine base
	Pyristine (piristina)
	Resistamine
	Tonaril
	Tripelannamine
	Tripelenamine
	Tripelennamin
	Tripelennamina
	Tripellenamine
	Triplennamine
	«beta»-Dimethylaminoethyl-2-pyridylaminotoluene
	«beta»-Dimethylaminoethyl-2-pyridylbenzylamine
	Â«betaÂ»-Dimethylaminoethyl-2-pyridylaminotoluene
	Â«betaÂ»-Dimethylaminoethyl-2-pyridylbenzylamine
Inchi:	InChI=1S/C16H21N3/c1-18(2)12-13-19(16-10-6-7-11-17-16)14-15-8-4-3-5-9-15/h3-11H,1
InchiKey:	UFLGIAIHIAPJJC-UHFFFAOYSA-N
Formula:	C16H21N3
SMILES:	CN(C)CCN(Cc1ccccc1)c1ccccn1

Mol. weight [g/mol]: 255.36
CAS: 91-81-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Aqueous Solubility Prediction Method
logp	2.650		Crippen Method
mcvol	218.720	ml/mol	McGowan Method
rinpol	1974.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1976.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1976.00		NIST Webbook
rinpol	1970.00		NIST Webbook
rinpol	1961.00		NIST Webbook
ripol	2682.00		NIST Webbook
ripol	2682.00		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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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