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	1975.00		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	1974.00		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
rinpol	1980.00		NIST Webbook
rinpol	1974.00		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