

1-Piperazineethanamine, N,N,4-trimethyl-

Other names:	N-Methyl-N'-(«beta»-dimethylaminoethyl)piperazine N-Methyl-N'-(dimethylaminoethyl)piperazine S 36081-3 1-(2-(Dimethylamino)ethyl)-4-methylpiperazine 1-(2-(N,N-Dimethylamino)ethyl)-4-methylpiperazine Piperazine, 1-[2-(dimethylamino)ethyl]-4-methyl- Kaolizer 8 NSC 79879 Toyocat NP N,N,4-trimethylpiperazine-1-ethylamine
Inchi:	InChI=1S/C9H21N3/c1-10(2)4-7-12-8-5-11(3)6-9-12/h4-9H2,1-3H3
InchiKey:	XFLSMWXCZBIXLV-UHFFFAOYSA-N
Formula:	C9H21N3
SMILES:	CN(C)CCN1CCN(C)CC1
Mol. weight [g/mol]:	171.28
CAS:	104-19-8

Physical Properties

Property code	Value	Unit	Source
log10ws	0.81		Crippen Method
logp	-0.205		Crippen Method
mcvol	156.750	ml/mol	McGowan Method
tf	220.30 ± 0.60	K	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104198&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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