

1-Piperazinecarboxamide, N,N-diethyl-4-methyl-

Other names:	Diethylcarbamazine
	Bitirazine
	Caracide
	Carbamazine
	Carbilazine
	Caricide
	Cypip
	Ditrazine base
	Ethodryl
	Notezine
	R.P. 3799
	RP 3799
	Spatonin
	1-Diethylcarbamoyl-4-methylpiperazine
	1-Diethylcarbamoyl-4-methylpiperzine
	1-Methyl-4-diethylcarbamoylpiperazine
	84L
	1-(N,N-Diethylcarbamoyl)-4-methylpiperazine
	N,N-Diethyl-4-methyl-1-piperazinecarboxamide
Inchi:	InChI=1S/C10H21N3O/c1-4-12(5-2)10(14)13-8-6-11(3)7-9-13/h4-9H2,1-3H3
InchiKey:	RCKMWOKWVGPNJF-UHFFFAOYSA-N
Formula:	C10H21N3O
SMILES:	CCN(CC)C(=O)N1CCN(C)CC1
Mol. weight [g/mol]:	199.29
CAS:	90-89-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.37		Crippen Method
logp	0.696		Crippen Method
mcvol	172.410	ml/mol	McGowan Method
tf	322.37 ± 0.40	K	NIST Webbook
tf	322.75 ± 0.20	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.20	K	0.40	NIST Webbook
tbrp	413.00 ± 1.00	K	1.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90891&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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