N,N-DIETHYL-4-METHYL-1-PIPERAZINECARBOX

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]:	199.30

Physical Properties

Property code	Value	Unit	Source
log10ws	1.18		Cheméo Relay (1.0)
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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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