1,4-Pentanediamine, N1,N1-diethyl-

Other names:	1-(Diethylamino)-4-aminopentane
	1-Methyl-4-(diethylamino)butylamine
	1-Methyl-4-dietylaminobutylamine
	2-Amino-5-(diethylamino)pentane
	4-(Diethylamino)-1-methylbutylamine
	4-Amino-1-(diethylamino)pentane
	4-aminopentyldiethylamine
	5-(Diethylamino)-2-pentylamine
	5-Diethylamino-2-aminopentane
	N,N-Diethyl-1,4-pentanediamine
	N,N-Diethyl-4-methyltetramethylenediamine
	N1,N1-Diethyl-1,4-pentanediamine
	N5,N5-Diethyl-2,5-pentanediamine
	NSC 2606
	Novoldiamine
	Tetramethylenediamine, N,N-diethyl-4-methyl-
	«delta»-(Diethylamino)-«alpha»-methylbutylamine
	«delta»-Diethylaminoisopentylamine
	Â«deltaÂ»-(Diethylamino)-Â«alphaÂ»-methylbutylamine
	Â«deltaÂ»-Diethylaminoisopentylamine
Inchi:	InChI=1S/C9H22N2/c1-4-11(5-2)8-6-7-9(3)10/h9H,4-8,10H2,1-3H3
InchiKey:	CAPCBAYULRXQAN-UHFFFAOYSA-N
Formula:	C9H22N2
SMILES:	CCN(CC)CCCC(C)N
Mol. weight [g/mol]:	158.28
CAS:	140-80-7

Physical Properties

Property code	Value	Unit	Source
gf	199.69	kJ/mol	Joback Method
hf	-133.05	kJ/mol	Joback Method
hfus	23.76	kJ/mol	Joback Method
hvap	47.92	kJ/mol	Joback Method
log10ws	-1.71		Crippen Method
logp	1.456		Crippen Method
mcvol	157.630	ml/mol	McGowan Method
pc	2453.17	kPa	Joback Method

tb	489.85	K	Joback Method
tc	667.55	K	Joback Method
tf	291.92	K	Joback Method
vc	0.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.37	J/mol×K	489.85	Joback Method
cpg	386.06	J/mol×K	519.47	Joback Method
cpg	401.04	J/mol×K	549.08	Joback Method
cpg	415.34	J/mol×K	578.70	Joback Method
cpg	428.99	J/mol×K	608.32	Joback Method
cpg	441.99	J/mol×K	637.93	Joback Method
cpg	454.39	J/mol×K	667.55	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	473.70	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56863e+01
Coeff. B	-4.44030e+03
Coeff. C	-7.29640e+01
Temperature range (K), min.	361.32
Temperature range (K), max.	500.95

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C140807&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume