1-Nonanamine

Other names:	1-AMINONONANE
	1-Nonylamine
	Nonylamine
	n-Nonylamine
Inchi:	InChI=1S/C9H21N/c1-2-3-4-5-6-7-8-9-10/h2-10H2,1H3
InchiKey:	FJDUDHYHRVPMJZ-UHFFFAOYSA-N
Formula:	C9H21N
SMILES:	CCCCCCCCCN
Mol. weight [g/mol]:	143.27
CAS:	112-20-9

Physical Properties

Property code	Value	Unit	Source
basg	879.50 ± 9.20	kJ/mol	NIST Webbook
gf	91.35	kJ/mol	Joback Method
hf	-195.30	kJ/mol	Joback Method
hfus	24.26	kJ/mol	Joback Method
hvap	46.27	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method
logp	2.696		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	2438.65	kPa	Joback Method
rinpol	1133.00		NIST Webbook
rinpol	1141.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1412.00		NIST Webbook
ripol	1416.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1418.00		NIST Webbook
tb	475.35 ± 1.00	K	NIST Webbook
tb	475.40	K	NIST Webbook
tb	474.20	K	NIST Webbook
tc	653.68	K	Joback Method
tf	274.45	K	Joback Method
vc	0.569	m3/kmol	Joback Method

volm	1.83e-04	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	403.58	J/mol×K	624.37	Joback Method
cpg	336.56	J/mol×K	477.85	Joback Method
cpg	351.12	J/mol×K	507.15	Joback Method
cpg	365.09	J/mol×K	536.46	Joback Method
cpg	378.48	J/mol×K	565.76	Joback Method
cpg	391.30	J/mol×K	595.07	Joback Method
cpg	415.33	J/mol×K	653.68	Joback Method
hvapt	50.70	kJ/mol	427.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58005e+01
Coeff. B	-4.48296e+03
Coeff. C	-7.32970e+01
Temperature range (K), min.	362.28
Temperature range (K), max.	500.69

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.34706e+02
Coeff. B	-1.17243e+04
Coeff. C	-1.74800e+01
Coeff. D	1.03005e-05
Temperature range (K), min.	273.15
Temperature range (K), max.	648.00

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1276.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112209&Units=SI
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1276
Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K:	https://www.doi.org/10.1016/j.jct.2010.12.025
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

basg:	Gas basicity
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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
volm:	Molar Volume

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