N-Allyl-N,N-dimethylamine

Other names:	2-Propen-1-amine, N,N-dimethyl- Allylamine, N,N-dimethyl- Allyldimethylamine CH2=CHCH2N(CH3)2 Dimethylallylamine N,N-Dimethyl-2-propene-1-amine N,N-Dimethylallylamine N-Allyldimethylamine
Inchi:	InChI=1S/C5H11N/c1-4-5-6(2)3/h4H,1,5H2,2-3H3
InchiKey:	GBCKRQRXNXQQPW-UHFFFAOYSA-N
Formula:	C5H11N
SMILES:	C=CCN(C)C
Mol. weight [g/mol]:	85.15
CAS:	2155-94-4

Physical Properties

Property code	Value	Unit	Source
affp	957.80	kJ/mol	NIST Webbook
basg	926.80	kJ/mol	NIST Webbook
gf	189.84	kJ/mol	Joback Method
hf	46.43	kJ/mol	Joback Method
hfus	10.45	kJ/mol	Joback Method
hvap	28.10	kJ/mol	Joback Method
ie	7.84 ± 0.05	eV	NIST Webbook
ie	7.84	eV	NIST Webbook
ie	7.84 ± 0.03	eV	NIST Webbook
log10ws	-0.34		Crippen Method
logp	0.734		Crippen Method
mcvol	86.990	ml/mol	McGowan Method
pc	3637.73	kPa	Joback Method
rinpol	604.00		NIST Webbook
rinpol	604.00		NIST Webbook
tb	335.15 ± 2.00	K	NIST Webbook
tb	336.70	K	NIST Webbook
tc	488.29	K	Joback Method
tf	176.82	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.30	J/mol×K	322.92	Joback Method
cpg	146.21	J/mol×K	350.48	Joback Method
cpg	155.69	J/mol×K	378.04	Joback Method
cpg	164.78	J/mol×K	405.60	Joback Method
cpg	173.47	J/mol×K	433.16	Joback Method
cpg	181.78	J/mol×K	460.72	Joback Method
cpg	189.72	J/mol×K	488.29	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51860e+01
Coeff. B	-3.19264e+03
Coeff. C	-3.45860e+01
Temperature range (K), min.	248.88
Temperature range (K), max.	357.91

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2155944&Units=SI

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

Legend

affp:	Proton affinity
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
ie:	Ionization energy
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume