2-Propen-1-amine

Other names:	2-Propenamine
	2-Propenylamine
	3-AMINO-1-PROPENE
	3-Aminopropene
	3-Aminopropylene
	Allylamine
	CH2=CHCH2NH2
	MONOALLYLAMINE
	NSC 7600
	UN 2334
Inchi:	InChI=1S/C3H7N/c1-2-3-4/h2H,1,3-4H2
InchiKey:	VVJKKWFAADXIJK-UHFFFAOYSA-N
Formula:	C3H7N
SMILES:	C=CCN
Mol. weight [g/mol]:	57.09
CAS:	107-11-9

Physical Properties

Property code	Value	Unit	Source
affp	909.50	kJ/mol	NIST Webbook
basg	875.50	kJ/mol	NIST Webbook
chl	-2204.00	kJ/mol	NIST Webbook
gf	128.67	kJ/mol	Joback Method
hf	53.97	kJ/mol	Joback Method
hfl	10.00	kJ/mol	NIST Webbook
hfus	7.44	kJ/mol	Joback Method
hvap	32.24	kJ/mol	Joback Method
ie	8.76	eV	NIST Webbook
ie	9.40 ± 0.30	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
log10ws	-0.37		Crippen Method
logp	0.131		Crippen Method
mcvol	58.810	ml/mol	McGowan Method
pc	5051.40	kPa	Joback Method
rinpol	463.00		NIST Webbook
rinpol	468.00		NIST Webbook
rinpol	463.00		NIST Webbook

rinpol	463.00		NIST Webbook
rinpol	463.00		NIST Webbook
rinpol	468.00		NIST Webbook
tb	331.20	K	NIST Webbook
tb	326.20	K	NIST Webbook
tb	326.45 ± 1.00	K	NIST Webbook
tc	523.28	K	Joback Method
tf	205.07	K	Joback Method
vc	0.213	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	93.82	J/mol×K	337.25	Joback Method
cpg	100.19	J/mol×K	368.25	Joback Method
cpg	106.27	J/mol×K	399.26	Joback Method
cpg	112.08	J/mol×K	430.26	Joback Method
cpg	117.63	J/mol×K	461.27	Joback Method
cpg	122.92	J/mol×K	492.27	Joback Method
cpg	127.96	J/mol×K	523.28	Joback Method
hvapt	33.00	kJ/mol	288.00	NIST Webbook
hvapt	32.60	kJ/mol	298.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48898e+01
Coeff. B	-2.93985e+03
Coeff. C	-3.99840e+01
Temperature range (K), min.	241.31
Temperature range (K), max.	347.25

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	6.67682e+01
Coeff. B	-5.95608e+03
Coeff. C	-7.69122e+00
Coeff. D	5.62696e-06
Temperature range (K), min.	184.95
Temperature range (K), max.	505.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1319
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1319.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107119&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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