Aziridine, 2-methyl-

Other names:	1,2-PROPYLENIMINE
	1,2-Propyleneimine
	2-METHYLAZIRIDINE
	2-Methylazacyclopropane
	2-Methylethylenimine
	DL-2-methylaziderine
	Methylaziridine
	Methylethylenimine
	NSC 20655
	PROPYLENEIMINE
	PROPYLENIMINE
	Rcra waste number P067
Inchi:	InChI=1S/C3H7N/c1-3-2-4-3/h3-4H,2H2,1H3
InchiKey:	OZDGMOYKSFPLSE-UHFFFAOYSA-N
Formula:	C3H7N
SMILES:	CC1CN1
Mol. weight [g/mol]:	57.09
CAS:	75-55-8

Physical Properties

Property code	Value	Unit	Source
affp	925.10	kJ/mol	NIST Webbook
basg	892.10	kJ/mol	NIST Webbook
gf	122.84	kJ/mol	Joback Method
hf	5.36	kJ/mol	Joback Method
hfus	11.25	kJ/mol	Joback Method
hvap	28.94	kJ/mol	Joback Method
ie	9.57 ± 0.02	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
log10ws	-0.27		Crippen Method
logp	-0.022		Crippen Method
mcvol	52.250	ml/mol	McGowan Method
pc	5478.85	kPa	Joback Method
rinpol	618.00		NIST Webbook
tb	339.70	K	NIST Webbook
tc	513.92	K	Joback Method
tf	215.15 ± 0.60	K	NIST Webbook

vc	0.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	113.07	J/mol×K	482.16	Joback Method
cpg	76.50	J/mol×K	323.33	Joback Method
cpg	84.59	J/mol×K	355.10	Joback Method
cpg	92.28	J/mol×K	386.86	Joback Method
cpg	99.58	J/mol×K	418.63	Joback Method
cpg	106.50	J/mol×K	450.39	Joback Method
cpg	119.30	J/mol×K	513.92	Joback Method
rhol	802.23	kg/m3	298.20	The choice of solvent and liquid liquid equilibrium for ternary water + 2-methylaziridine + chloroform system: Experimental data and modeling

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	8.94820e+00
Coeff. B	-1.77133e+03
Coeff. C	-4.06050e+01
Temperature range (K), min.	229.00
Temperature range (K), max.	527.67

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.49572e+01
Coeff. B	-5.85689e+03

Coeff. C	-7.47620e+00
Coeff. D	5.66433e-06
Temperature range (K), min.	229.00
Temperature range (K), max.	529.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The choice of solvent and liquid liquid equilibrium for ternary water + 2-methylaziridine + chloroform system: Experimental data and modeling:	https://www.doi.org/10.1016/j.fluid.2012.11.018
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75558&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
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1335
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1335
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
rhol:	Liquid Density
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume