Ethylenimine

Other names:	1H-Azirine, dihydro-
	AZACYCLOPROPANE
	AZIRIDINE
	Aethylenimin
	Aziran
	Azirane
	Aziridin
	DIMETHYLENIMINE
	Dihydro-1H-azirine
	Dihydroazirene
	Dimethyleneimine
	EI
	ENT-50324
	Ethyleenimine
	Ethyleneimine
	Etilenimina
	Rcra waste number P054
	TL 337
	dihydroazirine
	perhydroazirine
Inchi:	InChI=1S/C2H5N/c1-2-3-1/h3H,1-2H2
InchiKey:	NOWKCMXCCJGMRR-UHFFFAOYSA-N
Formula:	C2H5N
SMILES:	C1CN1
Mol. weight [g/mol]:	43.07
CAS:	151-56-4

Physical Properties

Property code	Value	Unit	Source
af	0.4350		KDB
affp	905.50	kJ/mol	NIST Webbook
basg	872.50	kJ/mol	NIST Webbook
chl	-1591.36 ± 0.57	kJ/mol	NIST Webbook
gf	122.13	kJ/mol	Joback Method
hf	46.34	kJ/mol	Joback Method
hfl	91.90 ± 0.59	kJ/mol	NIST Webbook
hfus	7.59	kJ/mol	Joback Method

hvap	27.03	kJ/mol	Joback Method
ie	9.85 ± 0.02	eV	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.94 ± 0.15	eV	NIST Webbook
ie	9.52	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.85	eV	NIST Webbook
ie	9.20 ± 0.10	eV	NIST Webbook
log10ws	0.26		Crippen Method
logp	-0.410		Crippen Method
mcvol	38.160	ml/mol	McGowan Method
nfpaf	%!d(float64=3)		KDB
nfpah	%!d(float64=3)		KDB
nfpas	%!d(float64=3)		KDB
pc	9950.00	kPa	KDB
rinpol	402.00		NIST Webbook
rinpol	400.00		NIST Webbook
ripol	903.00		NIST Webbook
ripol	933.00		NIST Webbook
tb	328.50 ± 0.50	K	NIST Webbook
tb	328.60	K	KDB
tb	329.00 ± 2.00	K	NIST Webbook
tb	328.65 ± 0.60	K	NIST Webbook
tc	524.00	K	KDB
tf	195.00	K	KDB
tf	195.15 ± 0.50	K	NIST Webbook
vc	0.142	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	46.10	J/mol×K	305.12	Joback Method
cpg	52.42	J/mol×K	336.99	Joback Method
cpg	58.35	J/mol×K	368.86	Joback Method
cpg	63.91	J/mol×K	400.72	Joback Method
cpg	69.13	J/mol×K	432.59	Joback Method
cpg	74.02	J/mol×K	464.46	Joback Method
cpg	78.60	J/mol×K	496.33	Joback Method
hvapt	32.05	kJ/mol	328.60	KDB
hvapt	57.00 ± 0.20	kJ/mol	288.00	NIST Webbook
hvapt	34.90	kJ/mol	288.50	NIST Webbook

pvap	8.55	kPa	274.52	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	12.79	kPa	281.70	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	14.68	kPa	284.42	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	16.88	kPa	287.12	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	17.94	kPa	288.29	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	19.52	kPa	289.96	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	22.99	kPa	293.28	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	25.57	kPa	295.50	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	28.82	kPa	298.10	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	36.47	kPa	303.28	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44706e+01
Coeff. B	-2.70896e+03
Coeff. C	-5.35410e+01
Temperature range (K), min.	244.54
Temperature range (K), max.	349.98

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	7.49309e+01
Coeff. B	-6.49795e+03
Coeff. C	-8.81362e+00
Coeff. D	4.82903e-06
Temperature range (K), min.	195.20
Temperature range (K), max.	537.00

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C151564&Units=SI
Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with	https://www.doi.org/10.1016/j.jct.2011.04.017
Vapor Pressure and Its Temperature Dependence of 28 Organic	https://www.doi.org/10.1021/acs.jced.6b00576
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1334.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1334

Legend

af:	Acentric Factor
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
nfpas:	NFPA Safety Rating
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