Azetidine

Other names:	1,3-Propylenimine Azete, tetrahydro- Trimethylene imine Trimethylenimine azacyclobutane trimethyleneimine
Inchi:	InChI=1S/C3H7N/c1-2-4-3-1/h4H,1-3H2
InchiKey:	HONIICLYMWZJFZ-UHFFFAOYSA-N
Formula:	C3H7N
SMILES:	C1CNC1
Mol. weight [g/mol]:	57.09
CAS:	503-29-7

Physical Properties

Property code	Value	Unit	Source
affp	943.40	kJ/mol	NIST Webbook
basg	908.60	kJ/mol	NIST Webbook
gf	118.45	kJ/mol	Joback Method
hf	19.54	kJ/mol	Joback Method
hfus	8.08	kJ/mol	Joback Method
hvap	29.42	kJ/mol	Joback Method
ie	8.63 ± 0.02	eV	NIST Webbook
ie	8.30	eV	NIST Webbook
ie	8.90	eV	NIST Webbook
ie	9.10 ± 0.15	eV	NIST Webbook
ie	9.04 ± 0.02	eV	NIST Webbook
log10ws	-0.16		Crippen Method
logp	-0.020		Crippen Method
mcvol	52.250	ml/mol	McGowan Method
pc	5981.40	kPa	Joback Method
rinpol	599.00		NIST Webbook
tb	334.70	K	NIST Webbook
tb	336.00	K	NIST Webbook
tc	532.79	K	Joback Method
tf	247.26	K	Joback Method
vc	0.191	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	72.31	J/mol×K	332.27	Joback Method
cpg	81.03	J/mol×K	365.69	Joback Method
cpg	89.28	J/mol×K	399.11	Joback Method
cpg	97.07	J/mol×K	432.53	Joback Method
cpg	104.44	J/mol×K	465.95	Joback Method
cpg	111.40	J/mol×K	499.37	Joback Method
cpg	117.97	J/mol×K	532.79	Joback Method
hvapt	32.60	kJ/mol	288.00	NIST Webbook
pvap	6.51	kPa	273.18	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	8.22	kPa	277.55	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	9.69	kPa	280.44	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	10.89	kPa	282.64	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	14.18	kPa	288.04	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	14.22	kPa	288.04	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	18.88	kPa	293.56	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	
pvap	23.36	kPa	298.08	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols	

pvap	29.73	kPa	303.53	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C503297&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic study of (heptane + amine) mixtures. III: Excess and partial molar volumes in mixtures with secondary, tertiary, and cyclic amines at 298.15 K:	https://www.doi.org/10.1016/j.jct.2011.04.017
Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols:	https://www.doi.org/10.1021/acs.jced.6b00576

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
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