Azocine, octahydro-

Other names:	Azacyclooctane
	Heptamethyleneimine
	Heptamethylenimine
	Octahydroazocine
	Perhydroazocine
Inchi:	InChI=1S/C7H15N/c1-2-4-6-8-7-5-3-1/h8H,1-7H2
InchiKey:	QXNDZONIWRINJR-UHFFFAOYSA-N
Formula:	C7H15N
SMILES:	C1CCCNCCC1
Mol. weight [g/mol]:	113.20
CAS:	1121-92-2

Physical Properties

Property code	Value	Unit	Source
gf	103.73	kJ/mol	Joback Method
hf	-87.66	kJ/mol	Joback Method
hfus	10.04	kJ/mol	Joback Method
hvap	39.02	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.540		Crippen Method
mcvol	108.610	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
rinpol	938.00		NIST Webbook
tb	440.87	K	Joback Method
tc	670.82	K	Joback Method
tf	278.26	K	Joback Method
vc	0.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.04	J/mol×K	440.87	Joback Method
cpg	231.55	J/mol×K	479.20	Joback Method
cpg	249.13	J/mol×K	517.52	Joback Method

cpg	265.79	J/mol×K	555.85	Joback Method
cpg	281.54	J/mol×K	594.17	Joback Method
cpg	296.38	J/mol×K	632.50	Joback Method
cpg	310.31	J/mol×K	670.82	Joback Method
cpl	230.00	J/mol×K	298.00	NIST Webbook
hvapt	46.50	kJ/mol	293.00	NIST Webbook
pvap	0.42	kPa	299.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.11	kPa	279.60	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.13	kPa	281.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.17	kPa	285.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.22	kPa	288.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.28	kPa	292.10	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.27	kPa	292.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.33	kPa	295.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.42	kPa	299.00	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.09	kPa	276.10	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.52	kPa	302.10	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.69	kPa	306.10	Vapour pressure and enthalpy of vaporization of cyclic imines

pvap	0.83	kPa	309.00	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.79	kPa	309.00	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	1.02	kPa	313.00	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	1.31	kPa	317.00	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	1.44	kPa	319.80	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	1.58	kPa	322.00	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	1.97	kPa	324.90	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.07	kPa	273.22	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.12	kPa	279.40	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	0.16	kPa	284.11	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.21	kPa	287.87	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.30	kPa	293.35	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.40	kPa	297.82	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	0.56	kPa	302.95	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

pvap	0.75	kPa	308.09	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols
pvap	1.01	kPa	313.50	Vapor Pressure and Its Temperature Dependence of 28 Organic Compounds: Cyclic Amines, Cyclic Ethers, and Cyclic and Open Chain Secondary Alcohols

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	325.20	K	2.00	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
Computational assessment of thermodynamics of tautomerization of cyclic imines:	https://www.doi.org/10.1016/j.tca.2018.07.016
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1121922&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermodynamic study of heptane + amine mixtures. V. Excess and solvation Gibbs energies:	https://www.doi.org/10.1016/j.fluid.2014.12.017
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume