octamethylenimine

Other names:	azacyclononane
	azonane
	octahydro-1H-azonine
Inchi:	InChI=1S/C8H17N/c1-2-4-6-8-9-7-5-3-1/h9H,1-8H2
InchiKey:	NRHDCQLCSOWVTF-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	C1CCCCNCCC1
Mol. weight [g/mol]:	127.23

Physical Properties

Property code	Value	Unit	Source
gf	100.05	kJ/mol	Joback Method
hf	-114.46	kJ/mol	Joback Method
hfus	10.53	kJ/mol	Joback Method
hvap	41.41	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	1.930		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	468.02	K	Joback Method
tc	703.69	K	Joback Method
tf	286.01	K	Joback Method
vc	0.430	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.59	J/mol×K	468.02	Joback Method
cpg	277.42	J/mol×K	507.30	Joback Method
cpg	297.17	J/mol×K	546.58	Joback Method
cpg	315.84	J/mol×K	585.85	Joback Method
cpg	333.43	J/mol×K	625.13	Joback Method
cpg	349.94	J/mol×K	664.41	Joback Method
cpg	365.38	J/mol×K	703.69	Joback Method

pvap	0.03	kPa	283.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.02	kPa	278.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.01	kPa	274.60	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.04	kPa	288.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.05	kPa	293.20	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.07	kPa	298.10	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.12	kPa	304.10	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.17	kPa	309.10	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.21	kPa	313.30	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.28	kPa	318.10	Vapour pressure and enthalpy of vaporization of cyclic imines
pvap	0.39	kPa	323.40	Vapour pressure and enthalpy of vaporization of cyclic imines

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Vapour pressure and enthalpy of vaporization of cyclic imines:	https://www.doi.org/10.1016/j.tca.2018.07.016
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume