1,8-Diaminooctane

Other names:	1,8-Octamethylenediamine
	1,8-Octanediamine
	1,8-Octylenediamine
	Octamethylenediamine
Inchi:	InChI=1S/C8H20N2/c9-7-5-3-1-2-4-6-8-10/h1-10H2
InchiKey:	PWGJDPKCLMLPJW-UHFFFAOYSA-N
Formula:	C8H20N2
SMILES:	NCCCCCCCCN
Mol. weight [g/mol]:	144.26
CAS:	373-44-4

Physical Properties

Property code	Value	Unit	Source
basg	946.00 ± 21.00	kJ/mol	NIST Webbook
gf	149.38	kJ/mol	Joback Method
hf	-140.87	kJ/mol	Joback Method
hfus	65.94	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	65.26	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	65.42	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	65.42	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	64.89	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	64.90	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	65.63	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	68.56	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	68.19	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	68.04	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	67.82	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	67.46	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	67.09	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	67.00	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	66.72	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	50.51	kJ/mol	Solid-Liquid Equilibria of Naphthalene + Alkanediamine Mixtures
hfus	66.36	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	66.30	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	66.10	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	65.99	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	65.95	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	66.48	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hvap	54.68	kJ/mol	Joback Method
log10ws	-2.04		Crippen Method
logp	1.244		Crippen Method
mcvol	143.540	ml/mol	McGowan Method
pc	2800.00	kPa	Critical Pressures and Temperatures of n-Diaminoalkanes (C2 to C12)
rinpol	1273.00		NIST Webbook
ripol	1850.00		NIST Webbook
tb	498.70	K	NIST Webbook
tc	715.85	K	Joback Method
tf	346.44	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	353.74	J/mol×K	527.50	Joback Method
cpg	367.56	J/mol×K	558.89	Joback Method
cpg	380.74	J/mol×K	590.28	Joback Method
cpg	393.32	J/mol×K	621.67	Joback Method
cpg	405.30	J/mol×K	653.07	Joback Method
cpg	416.71	J/mol×K	684.46	Joback Method
cpg	427.57	J/mol×K	715.85	Joback Method
hfust	50.51	kJ/mol	324.90	NIST Webbook
hfust	50.98	kJ/mol	324.80	NIST Webbook
psub	6.80e-04	kPa	298.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	1.50e-04	kPa	288.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	1.50e-04	kPa	288.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	2.20e-04	kPa	290.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.20e-04	kPa	290.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.20e-04	kPa	290.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.20e-04	kPa	293.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.20e-04	kPa	293.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.20e-04	kPa	293.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	4.60e-04	kPa	295.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	4.60e-04	kPa	295.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	4.60e-04	kPa	295.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	1.50e-04	kPa	288.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	6.80e-04	kPa	298.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	6.80e-04	kPa	298.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	9.60e-04	kPa	300.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	9.60e-04	kPa	300.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	9.60e-04	kPa	300.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	1.40e-03	kPa	303.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	1.41e-03	kPa	303.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	1.40e-03	kPa	303.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.03e-03	kPa	306.00	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.03e-03	kPa	306.00	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.04e-03	kPa	306.00	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.98e-03	kPa	308.50	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.98e-03	kPa	308.50	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	2.98e-03	kPa	308.50	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	4.34e-03	kPa	311.01	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	4.32e-03	kPa	311.01	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	4.29e-03	kPa	311.01	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	6.27e-03	kPa	313.51	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	6.20e-03	kPa	313.51	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	6.25e-03	kPa	313.51	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	408.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56443e+01
Coeff. B	-4.62059e+03
Coeff. C	-7.96360e+01
Temperature range (K), min.	380.52
Temperature range (K), max.	526.81

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C373444&Units=SI
Solid-Liquid Equilibria of Naphthalene + Alkanediamine Mixtures:	https://www.doi.org/10.1021/je0502851
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Critical Pressures and Temperatures of n-Diaminoalkanes (C2 to C12):	https://www.doi.org/10.1021/je050424e
Activity Coefficients at Infinite Dilution by GLC in Alkanediamines as Stationary Phases:	https://www.doi.org/10.1021/je200628n
Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties:	https://www.doi.org/10.1016/j.fluid.2014.03.013
Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines:	https://www.doi.org/10.1016/j.jct.2011.06.008
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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

Legend

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
hfust:	Enthalpy of fusion at a given temperature
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
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	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

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