1,5-Pentanediamine

Other names:	1,5-Diaminopentane
	1,5-Pentamethylenediamine
	Animal coniine
	Cadaverin
	Cadaverine
	H2N(CH2)5NH2
	Pentamethylenediamine
	Pentane-1,5-diamine
Inchi:	InChI=1S/C5H14N2/c6-4-2-1-3-5-7/h1-7H2
InchiKey:	VHRGRCVQAFMJIZ-UHFFFAOYSA-N
Formula:	C5H14N2
SMILES:	NCCCCCN
Mol. weight [g/mol]:	102.18
CAS:	462-94-2

Physical Properties

Property code	Value	Unit	Source
affp	980.30	kJ/mol	NIST Webbook
affp	1008.00	kJ/mol	NIST Webbook
affp	999.60	kJ/mol	NIST Webbook
basg	946.20	kJ/mol	NIST Webbook
gf	124.12	kJ/mol	Joback Method
hf	-78.95	kJ/mol	Joback Method
hfus	58.66	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	58.37	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	58.26	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	58.10	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	58.09	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	57.83	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	57.54	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	57.54	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	57.47	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	57.45	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	58.66	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	57.06	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	56.98	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	56.67	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	56.42	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	56.28	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	56.27	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	56.27	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	56.26	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	56.07	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.88	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.87	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.87	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.87	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.86	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.67	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	58.67	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.47	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.46	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.47	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.46	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.46	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.26	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	55.27	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.07	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.07	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	54.87	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	54.74	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	54.74	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	54.66	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	55.63	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	57.07	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hvap	48.01	kJ/mol	Joback Method
log10ws	-0.78		Crippen Method
logp	0.074		Crippen Method
mcvol	101.270	ml/mol	McGowan Method
pc	3985.56	kPa	Joback Method
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	1035.00		NIST Webbook
ripol	1537.00		NIST Webbook
ripol	1537.00		NIST Webbook
tb	452.20	K	NIST Webbook
tb	451.65 ± 1.50	K	NIST Webbook
tb	452.65 ± 2.00	K	NIST Webbook
tc	654.01	K	Joback Method
tf	312.63	K	Joback Method
vc	0.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.81	J/mol×K	654.01	Joback Method
cpg	273.31	J/mol×K	621.48	Joback Method
cpg	264.39	J/mol×K	588.96	Joback Method
cpg	255.02	J/mol×K	556.43	Joback Method
cpg	245.19	J/mol×K	523.91	Joback Method
cpg	234.89	J/mol×K	491.38	Joback Method
cpg	224.09	J/mol×K	458.86	Joback Method
hfust	29.82	kJ/mol	285.00	NIST Webbook
psub	7.93e-03	kPa	278.48	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	7.84e-03	kPa	278.48	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	280.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	280.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	280.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	282.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	0.01	kPa	282.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.01	kPa	282.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	283.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	7.90e-03	kPa	278.48	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	283.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	284.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
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psub	0.02	kPa	286.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	286.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	286.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	5.48e-03	kPa	275.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	5.52e-03	kPa	275.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	5.53e-03	kPa	275.99	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

psub	3.88e-03	kPa	273.68	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.89e-03	kPa	273.68	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	3.90e-03	kPa	273.68	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties
psub	0.02	kPa	283.49	Thermodynamic study of alkane-alpha,omega-diamines - Evidence of odd-even pattern of sublimation properties

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C462942&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 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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1416.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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
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