1,11-Undecanediamine

Other names:	1,11-Diaminoundecane
	Undecamethylenediamine
	Undecane-1,11-diamine
Inchi:	InChI=1S/C11H26N2/c12-10-8-6-4-2-1-3-5-7-9-11-13/h1-13H2
InchiKey:	KLNPWTHGTVSSEU-UHFFFAOYSA-N
Formula:	C11H26N2
SMILES:	NCCCCCCCCCCCN
Mol. weight [g/mol]:	186.34
CAS:	822-08-2

Physical Properties

Property code	Value	Unit	Source
gf	174.64	kJ/mol	Joback Method
hf	-202.79	kJ/mol	Joback Method
hfus	80.32	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	79.92	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	79.53	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	79.35	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	79.15	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	80.70	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	78.75	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	78.57	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	78.37	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	77.98	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	77.59	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	78.96	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	81.09	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hvap	61.36	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	2.415		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
tb	596.14	K	Joback Method
tc	778.52	K	Joback Method
tf	380.25	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.28	J/mol×K	748.13	Joback Method
cpg	499.87	J/mol×K	596.14	Joback Method
cpg	515.77	J/mol×K	626.54	Joback Method
cpg	530.93	J/mol×K	656.93	Joback Method
cpg	545.39	J/mol×K	687.33	Joback Method
cpg	559.16	J/mol×K	717.73	Joback Method
cpg	584.76	J/mol×K	778.52	Joback Method
hfust	48.08	kJ/mol	313.60	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C822082&Units=SI

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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