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

Physical Properties

Property code	Value	Unit	Source
af	0.7682		Cheméo Relay (1.0)
gf	174.64	kJ/mol	Joback Method
hf	-235.56	kJ/mol	Cheméo Relay (1.0)
hfus	78.96	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	81.09	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	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	77.59	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	77.98	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
hvap	84.45	kJ/mol	Cheméo Relay (1.0)
ie	8.44	eV	Cheméo Relay (1.0)
log10ws	-3.94		Cheméo Relay (1.0)
logp	2.415		Crippen Method
mcvol	185.810	ml/mol	McGowan Method
pc	2143.35	kPa	Joback Method
tb	558.14	K	Cheméo Relay (1.0)
tc	742.57	K	Cheméo Relay (1.0)
tf	338.09	K	Cheméo Relay (1.0)
vc	0.719	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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	572.28	J/mol×K	748.13	Joback Method
cpg	584.76	J/mol×K	778.52	Joback Method
hfust	48.08	kJ/mol	313.60	NIST Webbook

Sources

Cheméo Relay (1.0, beta):	
Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines:	https://www.doi.org/10.1016/j.jct.2011.06.008
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C822082&Units=SI
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
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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