1,1O-DIAMINODECANE

Other names:	1,10-Decamethylenediamine
	1,10-Decanediamine
	1,10-Decylenediamine
	1,10-diaminodecane
	Decyldiamine
	decamethylenediamine
Inchi:	InChI=1S/C10H24N2/c11-9-7-5-3-1-2-4-6-8-10-12/h1-12H2
InchiKey:	YQLZOAVZWJBZSY-UHFFFAOYSA-N
Formula:	C10H24N2
SMILES:	NCCCCCCCCCCN
Mol. weight [g/mol]:	172.32

Physical Properties

Property code	Value	Unit	Source
af	0.7331		Cheméo Relay (1.0)
basg	946.00 ± 21.00	kJ/mol	NIST Webbook
gf	166.22	kJ/mol	Joback Method
hf	-213.50	kJ/mol	Cheméo Relay (1.0)
hfus	74.04	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	73.86	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	73.49	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	73.50	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	73.62	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	73.67	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines

hfus	73.80	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	73.98	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	74.10	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	74.22	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	74.41	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	75.33	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	75.32	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	75.13	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	75.01	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	74.95	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	74.77	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	74.71	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	74.59	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hfus	74.40	kJ/mol	Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines
hvap	79.23	kJ/mol	Cheméo Relay (1.0)
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-3.46		Cheméo Relay (1.0)

logp	2.025		Crippen Method
mcvol	171.720	ml/mol	McGowan Method
pc	2430.00	kPa	Critical Pressures and Temperatures of n-Diaminoalkanes (C2 to C12)
rinpol	1476.00		NIST Webbook
ripol	2061.00		NIST Webbook
ripol	2061.00		NIST Webbook
tb	543.56	K	Cheméo Relay (1.0)
tc	731.86	K	Cheméo Relay (1.0)
tf	331.89	K	Cheméo Relay (1.0)
vc	0.661	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.50	J/mol×K	573.26	Joback Method
cpg	464.79	J/mol×K	603.96	Joback Method
cpg	479.37	J/mol×K	634.66	Joback Method
cpg	493.28	J/mol×K	665.35	Joback Method
cpg	506.53	J/mol×K	696.05	Joback Method
cpg	519.15	J/mol×K	726.75	Joback Method
cpg	531.16	J/mol×K	757.45	Joback Method
hfust	57.81	kJ/mol	332.90	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	413.20	K	1.60	NIST Webbook

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vapor pressure and enthalpy of vaporization of linear aliphatic alkanediamines:	https://www.doi.org/10.1016/j.jct.2011.06.008
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):	
Activity Coefficients at Infinite Dilution by GLC in Alkanediamines as Stationary Phases:	https://www.doi.org/10.1021/je200628n
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C646253&Units=SI
Cheméo Relay (1.0, beta):	
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Critical Pressures and Temperatures of n-Diaminoalkanes (C2 to C12):	https://www.doi.org/10.1021/je050424e

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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