1,2-DIAMINO-2-METHYLPROPANE

Other names: 1,2-propanediamine, 2-methyl-
2,2-dimethylethylenediamine
2-methyl-1,2-diaminopropane
2-methyl-1,2-propanediamine
2-methylpropylenediamine
Methyl-2 propanediamine-1,2
Inchi: InChI=1S/C4H12N2/c1-4(2,6)3-5/h3,5-6H2,1-2H3
InchiKey: OPCJOXGBLDJWRM-UHFFFAOYSA-N
Formula: C4H12N2
SMILES: CC(C)(N)CN
Mol. weight [g/mol]: 88.15
CAS: 811-93-8

Physical Properties

Property code	Value	Unit	Source
chl	-3155.10 ± 0.59	kJ/mol	NIST Webbook
hf	-90.25 ± 0.71	kJ/mol	NIST Webbook
hfl	-134.00 ± 0.67	kJ/mol	NIST Webbook
hfus	9.10	kJ/mol	Joback Method
hvap	43.60 ± 0.20	kJ/mol	NIST Webbook
hvap	43.60 ± 0.20	kJ/mol	NIST Webbook
hvap	43.50 ± 0.20	kJ/mol	NIST Webbook
hvap	43.80	kJ/mol	NIST Webbook
hvap	43.50 ± 0.20	kJ/mol	NIST Webbook
ie	8.90	eV	Cheméo Relay (1.0)
logp	-0.318		Crippen Method
mcvol	87.180	ml/mol	McGowan Method
pc	4634.00	kPa	Joback Method
sl	259.53	J/mol×K	NIST Webbook
tb	388.19	K	Cheméo Relay (1.0)
tc	582.53	K	Cheméo Relay (1.0)
tf	249.40	K	Cheméo Relay (1.0)
tt	256.10 ± 0.20	K	NIST Webbook
tt	256.10 ± 0.20	K	NIST Webbook
vc	0.312	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	187.72	J/mol×K	432.75	Joback Method
cpg	198.45	J/mol×K	467.90	Joback Method
cpg	208.52	J/mol×K	503.05	Joback Method
cpg	217.95	J/mol×K	538.20	Joback Method
cpg	226.79	J/mol×K	573.35	Joback Method
cpg	235.06	J/mol×K	608.51	Joback Method
cpg	242.80	J/mol×K	643.66	Joback Method
cpl	234.56	J/mol×K	298.15	NIST Webbook
hfust	2.23	kJ/mol	256.10	NIST Webbook
hfust	2.23	kJ/mol	256.10	NIST Webbook
hfust	15.46	kJ/mol	237.50	NIST Webbook
hfust	2.23	kJ/mol	256.10	NIST Webbook
hvapt	47.20	kJ/mol	274.50	NIST Webbook
hvapt	47.20	kJ/mol	274.50	NIST Webbook
pvap	0.71	kPa	288.40	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.57	kPa	300.30	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.49	kPa	283.20	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.53	kPa	284.50	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.55	kPa	284.50	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study

pvap	0.59	kPa	286.00	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.46	kPa	282.40	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.80	kPa	290.40	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.92	kPa	292.50	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.05	kPa	294.30	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.14	kPa	295.90	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.30	kPa	297.20	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.42	kPa	299.00	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.48	kPa	282.40	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	1.75	kPa	302.00	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study

pvap	2.04	kPa	304.60	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	2.25	kPa	306.10	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	2.45	kPa	307.60	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	2.62	kPa	308.70	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.41	kPa	280.60	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.37	kPa	279.30	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.34	kPa	278.10	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.33	kPa	277.60	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.30	kPa	276.60	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
pvap	0.29	kPa	276.00	Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study
sfust	65.11	J/mol×K	237.50	NIST Webbook

sfust	8.71	J/mol×K	256.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.68884e+01
Coeff. B	-4.11103e+03
Coeff. C	-5.12800e+01
Temperature range (K), min.	298.92
Temperature range (K), max.	406.39

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Cheméo Relay (1.0):

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Benchmark thermodynamic properties of alkanediamines: Experimental and theoretical study: https://www.doi.org/10.1016/j.jct.2015.03.011

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C811938&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

chl: Standard liquid enthalpy of combustion

cpg: Ideal gas heat capacity

cpl: Liquid phase heat capacity

hf: Enthalpy of formation at standard conditions

hfl: Liquid phase 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

hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume

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