

2-Methyl-1,2-propanediamine

Other names:	1,2-Diamino-2-methylpropane 1,2-Propanediamine, 2-methyl- 2,2-dimethylethylenediamine 2-methyl-1,2-diaminopropane 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
gf	118.54	kJ/mol	Joback Method
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	43.80	kJ/mol	NIST Webbook
hvap	43.60 ± 0.20	kJ/mol	NIST Webbook
hvap	43.50 ± 0.20	kJ/mol	NIST Webbook
hvap	43.60 ± 0.20	kJ/mol	NIST Webbook
log10ws	-0.48		Crippen Method
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	432.75	K	Joback Method
tc	643.66	K	Joback Method
tf	303.78	K	Joback Method
tt	256.10 ± 0.20	K	NIST Webbook
vc	0.306	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	226.79	J/mol×K	573.35	Joback Method
cpg	235.06	J/mol×K	608.51	Joback Method
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	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
hvapt	47.20	kJ/mol	274.50	NIST Webbook
pvap	2.62	kPa	308.70	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	0.29	kPa	276.00	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	0.33	kPa	277.60	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	0.37	kPa	279.30	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	0.46	kPa	282.40	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	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	0.71	kPa	288.40	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	1.57	kPa	300.30	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	
sfust	8.71	J/mol×K	256.10	NIST Webbook	
sfust	65.11	J/mol×K	237.50	NIST Webbook	

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
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

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=C811938&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
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
log10ws:	Log10 of Water solubility in mol/l
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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