2-Propanamine, 2-methyl-

Other names:	(1,1-dimethylethyl)amine
	1,1-DIMETHYLETHYLAMINE
	1,1-Dimethylethanamine
	1-Amino-1,1-dimethylethane
	2-AMINEISOBUTANE
	2-Amino-2-Methylpropane
	2-Aminoisobutane
	2-Methyl-2-aminopropane
	2-Methyl-2-propanamine
	2-Methyl-2-propylamine
	Butylamine, tert
	Butylamine, tertiary
	Erbumine
	NSC 9571
	TRIMETHYLAMINOMETHANE
	t-Butylamine
	tert-Butylamine
	tert-C4H9NH2
Inchi:	InChI=1S/C4H11N/c1-4(2,3)5/h5H2,1-3H3
InchiKey:	YBRBMKDOPFTVDT-UHFFFAOYSA-N
Formula:	C4H11N
SMILES:	CC(C)(C)N
Mol. weight [g/mol]:	73.14
CAS:	75-64-9

Physical Properties

Property code	Value	Unit	Source
affp	934.10	kJ/mol	NIST Webbook
basg	899.90	kJ/mol	NIST Webbook
chl	-2997.00	kJ/mol	NIST Webbook
chl	-2995.50 ± 0.42	kJ/mol	NIST Webbook
chl	-2995.80 ± 1.10	kJ/mol	NIST Webbook
gf	52.09	kJ/mol	Joback Method
hf	-120.30	kJ/mol	NIST Webbook
hf	-120.90 ± 0.63	kJ/mol	NIST Webbook
hf	-120.00 ± 0.80	kJ/mol	NIST Webbook
hf	-139.30	kJ/mol	NIST Webbook

hfl	-150.60 ± 0.50	kJ/mol	NIST Webbook
hfl	-150.00 ± 1.00	kJ/mol	NIST Webbook
hfl	-169.00	kJ/mol	NIST Webbook
hfus	3.90	kJ/mol	Joback Method
hvap	33.84	kJ/mol	Joback Method
ie	8.50 ± 0.10	eV	NIST Webbook
ie	8.64	eV	NIST Webbook
ie	8.83	eV	NIST Webbook
log10ws	-1.04		Crippen Method
logp	0.744		Crippen Method
mcvol	77.200	ml/mol	McGowan Method
pc	3840.00	kPa	KDB
pc	3840.00 ± 50.66	kPa	NIST Webbook
rhoc	250.13 ± 19.75	kg/m3	NIST Webbook
rinpol	501.00		NIST Webbook
rinpol	501.00		NIST Webbook
rinpol	501.00		NIST Webbook
rinpol	484.00		NIST Webbook
rinpol	432.00		NIST Webbook
rinpol	480.00		NIST Webbook
rinpol	435.00		NIST Webbook
rinpol	438.00		NIST Webbook
ripol	712.00		NIST Webbook
ripol	729.00		NIST Webbook
ripol	715.00		NIST Webbook
ripol	725.00		NIST Webbook
ripol	716.00		NIST Webbook
ripol	712.00		NIST Webbook
sl	233.63	J/mol×K	NIST Webbook
tb	317.19	K	KDB
tb	317.55	K	Vapor Liquid Equilibrium Data for Methanol + tert-Butylamine + N,N-Dimethylformamide and Constituent Binary Systems at Atmospheric Pressure
tc	483.90	K	KDB
tc	483.90 ± 0.50	K	NIST Webbook
tf	205.65 ± 1.50	K	NIST Webbook
tf	206.20	K	KDB
tt	206.21 ± 0.05	K	NIST Webbook
tt	206.19 ± 0.01	K	NIST Webbook
tt	206.19	K	KDB
vc	0.292	m3/kmol	KDB

volm	1.07e-04	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K
zc	0.2786900		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.85	J/mol×K	392.64	Joback Method
cpg	159.48	J/mol×K	425.06	Joback Method
cpg	168.57	J/mol×K	457.47	Joback Method
cpg	177.14	J/mol×K	489.89	Joback Method
cpg	185.22	J/mol×K	522.31	Joback Method
cpg	139.66	J/mol×K	360.22	Joback Method
cpg	192.84	J/mol×K	554.73	Joback Method
cpl	191.71	J/mol×K	298.15	NIST Webbook
cpl	192.00	J/mol×K	298.15	NIST Webbook
cpl	190.00	J/mol×K	298.15	NIST Webbook
hfust	0.88	kJ/mol	206.20	NIST Webbook
hvapt	28.27	kJ/mol	317.20	NIST Webbook
hvapt	30.10	kJ/mol	320.50	NIST Webbook
pvap	101.00	kPa	317.55	Vapor Liquid Equilibrium Data for Methanol + tert-Butylamine + N,N-Dimethylformamide and Constituent Binary Systems at Atmospheric Pressure
rhol	675.66	kg/m3	308.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model

rhol	681.18	kg/m3	303.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	686.65	kg/m3	298.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model
rhol	692.06	kg/m3	293.15	Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44182e+01
Coeff. B	-2.79208e+03
Coeff. C	-3.30890e+01
Temperature range (K), min.	206.19
Temperature range (K), max.	339.69

Sources

Solubility of N-tert-Butylbenzothiazole-2-sulfenamide in Several Pure and Binary Solvents:	https://www.doi.org/10.1021/acs.jced.8b00954
Vapor–Liquid Equilibrium Data for Methanol + tert-Butylamine + N,N-Dimethylformamide and Constituent Binary Systems at Atmospheric Pressure:	https://www.doi.org/10.1021/je201349k
Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K:	https://www.doi.org/10.1016/j.jct.2010.12.025

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1265.mol
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75649&Units=SI
Volumetric properties of binary mixtures of (acetonitrile + amines) at several temperatures with application of the ERAS model:	https://www.doi.org/10.1016/j.jct.2015.09.002
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

affp:	Proton affinity
basg:	Gas basicity
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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
volm:	Molar Volume
zc:	Critical Compressibility