2-Propanamine

Other names:	1-METHYLETHYLAMINE
	2-AMINOPROPANE
	2-Amino-propaan
	2-Amino-propano
	2-Aminopropan
	2-Propylamine
	Isopropilamina
	Isopropylamine
	Monoisopropylamine
	NSC 62775
	Propane, 2-amino-
	SEC-PROPYLAMINE
	UN 1221
	iso-C3H7NH2
	iso-Propylamine gas
Inchi:	InChI=1S/C3H9N/c1-3(2)4/h3H,4H2,1-2H3
InchiKey:	JJWLVOIRVHMVIS-UHFFFAOYSA-N
Formula:	C3H9N
SMILES:	CC(C)N
Mol. weight [g/mol]:	59.11
CAS:	75-31-0

Physical Properties

Property code	Value	Unit	Source
af	0.2910		KDB
affp	923.80	kJ/mol	NIST Webbook
aigt	675.37	K	KDB
basg	889.00	kJ/mol	NIST Webbook
chl	-2354.50 ± 0.50	kJ/mol	NIST Webbook
fll	2.30	% in Air	KDB
flu	12.00	% in Air	KDB
fpc	247.04	K	KDB
gf	38.39	kJ/mol	Joback Method
hf	-83.82	kJ/mol	KDB
hf	-83.76 ± 0.79	kJ/mol	NIST Webbook
hf	-83.70 ± 0.80	kJ/mol	NIST Webbook
hfl	-112.30 ± 0.67	kJ/mol	NIST Webbook

hfus	5.20	kJ/mol	Joback Method
hvap	28.40	kJ/mol	NIST Webbook
hvap	28.50 ± 0.20	kJ/mol	NIST Webbook
hvap	28.71	kJ/mol	NIST Webbook
hvap	28.50	kJ/mol	NIST Webbook
ie	9.31	eV	NIST Webbook
ie	8.60 ± 0.10	eV	NIST Webbook
ie	8.86	eV	NIST Webbook
ie	8.72 ± 0.03	eV	NIST Webbook
log10ws	-0.62		Crippen Method
logp	0.353		Crippen Method
mcvol	63.110	ml/mol	McGowan Method
nfpaf	%!d(float64=4)		KDB
nfpah	%!d(float64=3)		KDB
pc	4540.00	kPa	KDB
pc	4540.00 ± 50.66	kPa	NIST Webbook
rhoc	267.77 ± 0.01	kg/m3	NIST Webbook
rinpol	465.00		NIST Webbook
rinpol	469.00		NIST Webbook
rinpol	469.00		NIST Webbook
rinpol	477.00		NIST Webbook
rinpol	465.00		NIST Webbook
rinpol	468.00		NIST Webbook
rinpol	469.00		NIST Webbook
rinpol	465.00		NIST Webbook
ripol	743.00		NIST Webbook
ripol	725.00		NIST Webbook
ripol	740.00		NIST Webbook
ripol	710.00		NIST Webbook
ripol	743.00		NIST Webbook
ripol	740.00		NIST Webbook
sl	218.32	J/mol×K	NIST Webbook
tb	305.01 ± 0.25	K	NIST Webbook
tb	304.90	K	NIST Webbook
tb	305.55	K	NIST Webbook
tb	304.91	K	KDB
tb	307.15 ± 1.50	K	NIST Webbook
tb	305.15 ± 2.00	K	NIST Webbook
tb	306.15 ± 0.30	K	NIST Webbook
tb	304.65 ± 1.00	K	NIST Webbook
tb	307.15 ± 1.00	K	NIST Webbook
tb	306.70	K	NIST Webbook
tb	305.60	K	NIST Webbook
tc	471.90 ± 0.50	K	NIST Webbook

tc	471.80	K	NIST Webbook
tc	472.50	K	Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons
tc	471.80	K	KDB
tf	177.95	K	NIST Webbook
tf	171.95 ± 0.60	K	NIST Webbook
tf	178.01	K	KDB
tt	178.01 ± 0.01	K	NIST Webbook
vc	0.221	m3/kmol	KDB
volm	8.67e-05	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K
zc	0.2557720		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	134.01	J/mol×K	464.53	Joback Method
cpg	146.33	J/mol×K	526.73	Joback Method
cpg	140.30	J/mol×K	495.63	Joback Method
cpg	106.13	J/mol×K	340.13	Joback Method
cpg	113.52	J/mol×K	371.23	Joback Method
cpg	120.63	J/mol×K	402.33	Joback Method
cpg	127.46	J/mol×K	433.43	Joback Method
cpl	164.00	J/mol×K	313.00	NIST Webbook
cpl	164.00	J/mol×K	298.15	NIST Webbook
cpl	165.30	J/mol×K	298.15	NIST Webbook
cpl	163.85	J/mol×K	298.15	NIST Webbook
hfust	7.33	kJ/mol	178.00	NIST Webbook
hfust	7.33	kJ/mol	178.00	NIST Webbook
hfust	7.32	kJ/mol	177.99	NIST Webbook
hvapt	27.20	kJ/mol	313.00	NIST Webbook
hvapt	27.83	kJ/mol	304.90	NIST Webbook
hvapt	29.70	kJ/mol	305.50	NIST Webbook
rhol	683.94	kg/m3	298.15	Excess enthalpies of binary mixtures of some propylamines + some propanols at 298.15K
rhol	688.00	kg/m3	293.00	KDB

sfust	41.15	J/mol×K	177.99	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42286e+01
Coeff. B	-2.49064e+03
Coeff. C	-4.68340e+01
Temperature range (K), min.	225.49
Temperature range (K), max.	471.85

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.27941e+01
Coeff. B	-6.47623e+03
Coeff. C	-1.18881e+01
Coeff. D	1.14303e-05
Temperature range (K), min.	177.95
Temperature range (K), max.	471.85

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75310&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Gas-Liquid Critical Temperatures of Some Alkenes, Amines, and Cyclic Hydrocarbons:	https://www.doi.org/10.1021/je0341357
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1259.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
Thermodynamic study of heptane + amine mixtures. V. Excess and solvation Gibbs energies:	https://www.doi.org/10.1016/j.fluid.2014.12.017
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1259
Excess enthalpies of binary mixtures of some propylamines + some propanols at 298.15K:	https://www.doi.org/10.1016/j.tca.2006.08.006
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
affp:	Proton affinity
aigt:	Autoignition Temperature
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
fll:	Lower Flammability Limit
flu:	Upper Flammability Limit
fpc:	Flash Point (Closed Cup Method)
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
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure
pvap:	Vapor pressure
rhoc:	Critical density
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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
volm:	Molar Volume
zc:	Critical Compressibility