Isobutylamine

Other names:	(2-methylpropyl)amine
	1-Amino-2-methylpropane
	1-Propanamine, 2-methyl-
	2-Methyl-1-Aminopropane
	2-Methyl-1-propanamine
	2-Methylpropanamine
	2-Methylpropylamine
	3-Methyl-2-propylamine
	Monoisobutylamine
	NSC 8028
	UN 1214
	Valamine
	i-Butylamine
	iso-C4H9NH2
Inchi:	InChI=1S/C4H11N/c1-4(2)3-5/h4H,3,5H2,1-2H3
InchiKey:	KDSNLYIMUZNERS-UHFFFAOYSA-N
Formula:	C4H11N
SMILES:	CC(C)CN
Mol. weight [g/mol]:	73.14
CAS:	78-81-9

Physical Properties

Property code	Value	Unit	Source
affp	924.80	kJ/mol	NIST Webbook
basg	890.80	kJ/mol	NIST Webbook
chl	-2987.00	kJ/mol	NIST Webbook
chl	-3013.50 ± 0.42	kJ/mol	NIST Webbook
gf	46.81	kJ/mol	Joback Method
hf	-144.10	kJ/mol	NIST Webbook
hf	-98.62 ± 0.54	kJ/mol	NIST Webbook
hfl	-178.00	kJ/mol	NIST Webbook
hfl	-132.50 ± 0.50	kJ/mol	NIST Webbook
hfus	7.79	kJ/mol	Joback Method
hvap	34.75	kJ/mol	Joback Method
ie	8.50 ± 0.10	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
log10ws	-0.69		Crippen Method

logp	0.601		Crippen Method
mcvol	77.200	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
rinpol	591.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	588.00		NIST Webbook
rinpol	588.00		NIST Webbook
rinpol	591.00		NIST Webbook
rinpol	600.00		NIST Webbook
rinpol	605.00		NIST Webbook
rinpol	581.00		NIST Webbook
rinpol	548.00		NIST Webbook
rinpol	543.00		NIST Webbook
rinpol	591.00		NIST Webbook
ripol	842.00		NIST Webbook
ripol	855.00		NIST Webbook
ripol	840.00		NIST Webbook
ripol	842.00		NIST Webbook
ripol	842.00		NIST Webbook
ripol	860.00		NIST Webbook
tb	341.15 ± 1.50	K	NIST Webbook
tb	341.70	K	NIST Webbook
tb	342.00 ± 3.00	K	NIST Webbook
tb	341.65 ± 1.50	K	NIST Webbook
tb	341.15 ± 0.50	K	NIST Webbook
tb	341.15 ± 2.00	K	NIST Webbook
tb	340.15 ± 1.00	K	NIST Webbook
tb	340.85 ± 0.30	K	NIST Webbook
tb	340.70	K	NIST Webbook
tc	516.90	K	NIST Webbook
tf	187.65 ± 0.50	K	NIST Webbook
tf	188.55 ± 1.50	K	NIST Webbook
tf	186.50 ± 0.50	K	NIST Webbook
vc	0.282	m3/kmol	Joback Method
volm	1.01e-04	m3/mol	Thermodynamic study of (heptane + amine) mixtures. II. Excess and partial molar volumes at 298.15 K

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	187.35	J/mol×K	549.17	Joback Method
cpg	147.57	J/mol×K	394.04	Joback Method
cpg	156.20	J/mol×K	425.06	Joback Method
cpg	164.49	J/mol×K	456.09	Joback Method
cpg	172.44	J/mol×K	487.12	Joback Method
cpg	180.06	J/mol×K	518.14	Joback Method
cpg	138.58	J/mol×K	363.01	Joback Method
cpl	194.00	J/mol×K	298.15	NIST Webbook
hvapt	30.61	kJ/mol	340.70	NIST Webbook
hvapt	37.60	kJ/mol	297.50	NIST Webbook
hvapt	32.70 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	31.60 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	33.50	kJ/mol	318.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	6.78232e+01
Coeff. B	-6.17764e+03
Coeff. C	-7.84560e+00
Coeff. D	5.37349e-06
Temperature range (K), min.	188.55
Temperature range (K), max.	664.00

Sources

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

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

KDB: https://www.cheric.org/files/research/kdb/mol/mol1263.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C78819&Units=SI

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1263

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
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
volm:	Molar Volume