1-Butanamine, 3-methyl-

Other names:	1-Amino-3-methylbutane
	2-(2-Isopropyl)ethylamine
	3-Methylbutanamine
	3-Methylbutylamine
	3-methyl-1-butanamine
	Butylamine, 3-methyl-
	Isoamylamine
	Isopentylamine
	Isovalerylamine
	Leucamine
	Monoisoamylamine
	Monoisopentylamine
	NSC 7907
	Propylamine, 3,3-dimethyl-
	«gamma»-Isoamylamine
	Â«gammaÂ»-Isoamylamine
Inchi:	InChI=1S/C5H13N/c1-5(2)3-4-6/h5H,3-4,6H2,1-2H3
InchiKey:	BMFVGAAISNGQNM-UHFFFAOYSA-N
Formula:	C5H13N
SMILES:	CC(C)CCN
Mol. weight [g/mol]:	87.16
CAS:	107-85-7

Physical Properties

Property code	Value	Unit	Source
chl	-3639.00	kJ/mol	NIST Webbook
gf	55.23	kJ/mol	Joback Method
hf	-118.02	kJ/mol	Joback Method
hfl	-210.00	kJ/mol	NIST Webbook
hfus	10.38	kJ/mol	Joback Method
hvap	36.98	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	0.991		Crippen Method
mcvol	91.290	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	696.00		NIST Webbook
rinpol	696.00		NIST Webbook

rinpol	695.00		NIST Webbook
rinpol	695.00		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	698.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	698.00		NIST Webbook
ripol	989.00		NIST Webbook
tb	368.15 ± 3.00	K	NIST Webbook
tb	368.65 ± 3.00	K	NIST Webbook
tb	351.65 ± 5.00	K	NIST Webbook
tb	368.65 ± 4.00	K	NIST Webbook
tb	368.15 ± 3.00	K	NIST Webbook
tb	369.20	K	NIST Webbook
tc	571.20	K	Joback Method
tf	214.37	K	Joback Method
vc	0.339	m3/kmol	Joback Method
volm	1.17e-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	173.57	J/mol×K	385.89	Joback Method
cpg	184.03	J/mol×K	416.77	Joback Method
cpg	194.06	J/mol×K	447.66	Joback Method
cpg	203.68	J/mol×K	478.54	Joback Method
cpg	212.89	J/mol×K	509.43	Joback Method
cpg	221.72	J/mol×K	540.31	Joback Method
cpg	230.17	J/mol×K	571.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)

Coeff. A	1.44688e+01
Coeff. B	-2.76028e+03
Coeff. C	-8.57820e+01
Temperature range (K), min.	280.43
Temperature range (K), max.	387.21

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C107857&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
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/mol1391.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas 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
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