1-Butanamine, N,N-dimethyl-

Other names:	1-(N,N-Dimethylamino)butane
	Butylamine, N,N-dimethyl-
	Butyldimethylamine
	Dimethylbutylamine
	N,N-Dimethyl-1-butanamine
	N,N-Dimethyl-n-butylamine
	N,N-Dimethylbutylamine
	N,N-dimethylbutanamine
	N-n-Butyldimethylamine
	n-C4H9N(CH3)2
Inchi:	InChI=1S/C6H15N/c1-4-5-6-7(2)3/h4-6H2,1-3H3
InchiKey:	DJEQZVQFEPKLOY-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CCCCN(C)C
Mol. weight [g/mol]:	101.19
CAS:	927-62-8

Physical Properties

Property code	Value	Unit	Source
affp	969.20	kJ/mol	NIST Webbook
basg	938.20	kJ/mol	NIST Webbook
gf	110.42	kJ/mol	Joback Method
hf	-99.64	kJ/mol	Joback Method
hfus	14.32	kJ/mol	Joback Method
hvap	30.99	kJ/mol	Joback Method
ie	8.35	eV	NIST Webbook
log10ws	-0.90		Crippen Method
logp	1.348		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
rinpol	697.00		NIST Webbook
rinpol	697.00		NIST Webbook
rinpol	676.30		NIST Webbook
rinpol	696.00		NIST Webbook
rinpol	696.00		NIST Webbook
tb	366.65 ± 3.00	K	NIST Webbook
tb	365.65 ± 5.00	K	NIST Webbook

tb	366.65 ± 3.00	K	NIST Webbook
tb	366.00	K	NIST Webbook
tb	363.15 ± 3.00	K	NIST Webbook
tc	511.60	K	Joback Method
tf	189.85	K	Joback Method
vc	0.390	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.67	J/mol×K	376.20	Joback Method
cpg	207.01	J/mol×K	403.28	Joback Method
cpg	217.91	J/mol×K	430.36	Joback Method
cpg	228.39	J/mol×K	457.44	Joback Method
cpg	238.45	J/mol×K	484.52	Joback Method
cpg	183.89	J/mol×K	349.12	Joback Method
cpg	248.11	J/mol×K	511.60	Joback Method
pvap	29.84	kPa	330.90	Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT
pvap	49.84	kPa	345.00	Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT
pvap	69.83	kPa	355.10	Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT

pvap	89.83	kPa	363.20	Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT
pvap	99.83	kPa	366.70	Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.31970e+01
Coeff. B	-2.38465e+03
Coeff. C	-8.80240e+01
Temperature range (K), min.	272.75
Temperature range (K), max.	390.43

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Isobaric Vapor Liquid Equilibria of Tertiary Amine and n-Alkane/Alkanol Binary Mixtures: Experimental Measurements and Modeling with GC-PPC-SAFT: https://www.doi.org/10.1021/je300568h

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=C927628&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

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume