1-Butanamine, N-methyl-

Other names:	Butylamine, N-methyl-
	Butylmethylamine
	Methyl-N-butylamine
	Methylbutylamine
	N-Butyl-N-methylamine
	N-Butylmethylamine
	N-Methyl-n-butylamine
	N-Methylbutanamine
	N-Methylbutylamine
	UN 2945
	N-Methyl-1-butanamine
Inchi:	InChI=1S/C5H13N/c1-3-4-5-6-2/h6H,3-5H2,1-2H3
InchiKey:	QCOGKXLOEWLIDC-UHFFFAOYSA-N
Formula:	C5H13N
SMILES:	CCCCNC
Mol. weight [g/mol]:	87.16
CAS:	110-68-9

Physical Properties

Property code	Value	Unit	Source
chl	-3684.20 ± 3.70	kJ/mol	NIST Webbook
gf	80.61	kJ/mol	Joback Method
hf	-108.30 ± 4.30	kJ/mol	NIST Webbook
hfl	-141.20 ± 3.80	kJ/mol	NIST Webbook
hfus	13.80	kJ/mol	Joback Method
hvap	38.10	kJ/mol	NIST Webbook
hvap	32.90 ± 2.00	kJ/mol	NIST Webbook
hvap	32.90	kJ/mol	NIST Webbook
log10ws	-1.10		Crippen Method
logp	1.006		Crippen Method
mcvol	91.290	ml/mol	McGowan Method
pc	3522.09	kPa	Joback Method
rinpol	630.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	630.00		NIST Webbook
rinpol	601.00		NIST Webbook
tb	363.65 ± 3.00	K	NIST Webbook

tb	364.15 ± 0.60	K	NIST Webbook
tb	364.20	K	NIST Webbook
tb	364.25	K	NIST Webbook
tc	534.22	K	Joback Method
tf	198.15 ± 0.60	K	NIST Webbook
tf	198.20 ± 0.60	K	NIST Webbook
tf	198.15	K	NIST Webbook
vc	0.350	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	162.67	J/mol×K	363.97	Joback Method
cpg	172.76	J/mol×K	392.35	Joback Method
cpg	182.49	J/mol×K	420.72	Joback Method
cpg	191.86	J/mol×K	449.10	Joback Method
cpg	200.89	J/mol×K	477.47	Joback Method
cpg	209.56	J/mol×K	505.85	Joback Method
cpg	217.91	J/mol×K	534.22	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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=C110689&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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