2-Butanamine, N-(1-methylpropyl)-

Other names:	(sec-C4H9)2NH
	1-Propanamine, 1-methyl, N-(1-methylpropyl)
	Bis(1-methylpropyl)amine
	Di-sec-butylamine
	Di-sec.-butylamine
	MPBA
	N-(1-Methylpropyl)-2-butanamine
Inchi:	InChI=1S/C8H19N/c1-5-7(3)9-8(4)6-2/h7-9H,5-6H2,1-4H3
InchiKey:	OBYVIBDTOCAXSN-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CCC(C)NC(C)CC
Mol. weight [g/mol]:	129.24
CAS:	626-23-3

Physical Properties

Property code	Value	Unit	Source
affp	980.70	kJ/mol	NIST Webbook
basg	947.50	kJ/mol	NIST Webbook
chl	-5635.80 ± 2.30	kJ/mol	NIST Webbook
gf	100.99	kJ/mol	Joback Method
hf	-183.60 ± 3.00	kJ/mol	NIST Webbook
hfl	-227.70 ± 2.60	kJ/mol	NIST Webbook
hfus	14.53	kJ/mol	Joback Method
hvap	44.10 ± 1.50	kJ/mol	NIST Webbook
hvap	41.30 ± 0.30	kJ/mol	NIST Webbook
hvap	44.10	kJ/mol	NIST Webbook
ie	7.60	eV	NIST Webbook
log10ws	-2.58		Crippen Method
logp	2.173		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2611.07	kPa	Joback Method
rinpol	837.00		NIST Webbook
rinpol	837.00		NIST Webbook
tb	431.73	K	Joback Method
tc	607.62	K	Joback Method
tf	202.58	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.42	J/mol×K	431.73	Joback Method
cpg	293.82	J/mol×K	461.04	Joback Method
cpg	307.65	J/mol×K	490.36	Joback Method
cpg	320.91	J/mol×K	519.67	Joback Method
cpg	333.62	J/mol×K	548.99	Joback Method
cpg	345.79	J/mol×K	578.30	Joback Method
cpg	357.44	J/mol×K	607.62	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34117e+01
Coeff. B	-3.32541e+03
Coeff. C	-5.43380e+01
Temperature range (K), min.	307.72
Temperature range (K), max.	464.87

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=C626233&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
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
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

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