sec-Butylamine

Other names:	(.+/-.)-sec-Butylamine
	(RS)-2-aminobutane
	(RS)-sec-butylamine
	1-Methylpropanamine
	1-Methylpropylamine
	2-AB
	2-Aminobutane
	2-Aminobutane base
	2-Butanamine
	2-Butylamine
	Butafume
	Deccotane
	Frucote
	NSC 8030
	Propylamine, 1-Methyl-
	Secondary butylamine
	Tutane
	sec-Butanamine
	sec-C4H9NH2
Inchi:	InChI=1S/C4H11N/c1-3-4(2)5/h4H,3,5H2,1-2H3
InchiKey:	BHRZNVHARXXAHW-UHFFFAOYSA-N
Formula:	C4H11N
SMILES:	CCC(C)N
Mol. weight [g/mol]:	73.14
CAS:	13952-84-6

Physical Properties

Property code	Value	Unit	Source
affp	929.70	kJ/mol	NIST Webbook
basg	895.70	kJ/mol	NIST Webbook
chl	-2979.00	kJ/mol	NIST Webbook
chl	-3008.60 ± 0.92	kJ/mol	NIST Webbook
gf	46.81	kJ/mol	Joback Method
hf	-155.50	kJ/mol	NIST Webbook
hf	-106.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-137.50 ± 1.00	kJ/mol	NIST Webbook
hfl	-187.00	kJ/mol	NIST Webbook

hfus	7.79	kJ/mol	Joback Method
hvap	32.64 ± 0.06	kJ/mol	NIST Webbook
hvap	31.50	kJ/mol	NIST Webbook
hvap	31.00 ± 1.00	kJ/mol	NIST Webbook
hvap	32.70 ± 0.10	kJ/mol	NIST Webbook
hvap	32.60 ± 0.10	kJ/mol	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.50 ± 0.10	eV	NIST Webbook
log10ws	-1.04		Crippen Method
logp	0.744		Crippen Method
mcvol	77.200	ml/mol	McGowan Method
pc	5000.00 ± 499.79	kPa	NIST Webbook
rinpol	471.00		NIST Webbook
rinpol	527.00		NIST Webbook
rinpol	517.00		NIST Webbook
rinpol	515.00		NIST Webbook
rinpol	471.00		NIST Webbook
rinpol	471.00		NIST Webbook
rinpol	471.00		NIST Webbook
ripol	825.00		NIST Webbook
ripol	826.00		NIST Webbook
ripol	821.00		NIST Webbook
ripol	816.00		NIST Webbook
ripol	815.00		NIST Webbook
ripol	864.00		NIST Webbook
tb	336.15 ± 2.00	K	NIST Webbook
tb	336.15 ± 2.00	K	NIST Webbook
tb	336.15 ± 1.50	K	NIST Webbook
tb	336.00	K	NIST Webbook
tc	514.30 ± 0.51	K	NIST Webbook
tf	168.65 ± 0.60	K	NIST Webbook
vc	0.282	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	138.58	J/mol×K	363.01	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	187.35	J/mol×K	549.17	Joback Method
hvapt	34.10	kJ/mol	317.50	NIST Webbook
hvapt	32.40	kJ/mol	317.50	NIST Webbook
hvapt	31.60 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	30.50 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	29.40 ± 0.10	kJ/mol	343.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	5.75882e+01
Coeff. B	-5.56943e+03
Coeff. C	-6.33708e+00
Coeff. D	4.07040e-06
Temperature range (K), min.	168.65
Temperature range (K), max.	514.30

Sources

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=C13952846&Units=SI
KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1264
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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
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