2-Butanamine, (S)-

Other names: (+)-2-Butylamine
(S)-(+)-sec-Butylamine
(S)-sec-butylamine
S-2-Butylamine
sec-Butylamine, (S)-
Inchi: InChI=1S/C4H11N/c1-3-4(2)5/h4H,3,5H2,1-2H3/t4-/m1/s1
InchiKey: BHRZNVHARXXAHW-SCSAIBSYSA-N
Formula: C4H11N
SMILES: CCC(C)N
Mol. weight [g/mol]: 73.14
CAS: 513-49-5

Physical Properties

Property code	Value	Unit	Source
gf	46.81	kJ/mol	Joback Method
hf	-97.38	kJ/mol	Joback Method
hfus	7.79	kJ/mol	Joback Method
hvap	32.85	kJ/mol	NIST Webbook
log10ws	-1.04		Crippen Method
logp	0.744		Crippen Method
mcvol	77.200	ml/mol	McGowan Method
pc	4233.04	kPa	Joback Method
tb	336.20	K	NIST Webbook
tb	336.10	K	NIST Webbook
tc	509.40	K	NIST Webbook
tf	203.10	K	Joback Method
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	29.92	kJ/mol	336.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54689e+01
Coeff. B	-3.27571e+03
Coeff. C	-3.43080e+01
Temperature range (K), min.	250.08
Temperature range (K), max.	356.80

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=C513495&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

Legend

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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume