(S)-(+)-2-Amino-3-methyl-1-butanol

Other names:	(S)-2-Amino-3-methylbutanol
	1-Butanol, 2-amino-3-methyl-, (S)-
	L-2-amino-3-methylbutan-1-ol
	L-Valinol
Inchi:	InChI=1S/C5H13NO/c1-4(2)5(6)3-7/h4-5,7H,3,6H2,1-2H3/t5-/m0/s1
InchiKey:	NWYYWIJOWOLJNR-YFKPBYRVSA-N
Formula:	C5H13NO
SMILES:	CC(C)C(N)CO
Mol. weight [g/mol]:	103.16
CAS:	2026-48-4

Physical Properties

Property code	Value	Unit	Source
gf	-84.03	kJ/mol	Joback Method
hf	-275.53	kJ/mol	Joback Method
hfus	10.94	kJ/mol	Joback Method
hvap	53.27	kJ/mol	Joback Method
log10ws	-0.48		Crippen Method
logp	-0.038		Crippen Method
mcvol	97.160	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
tb	477.63	K	Joback Method
tc	659.47	K	Joback Method
tf	260.19	K	Joback Method
vc	0.351	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.41	J/mol×K	477.63	Joback Method
cpg	228.88	J/mol×K	507.94	Joback Method
cpg	237.94	J/mol×K	538.24	Joback Method
cpg	246.60	J/mol×K	568.55	Joback Method
cpg	254.87	J/mol×K	598.85	Joback Method

cpg	262.75	J/mol×K	629.16	Joback Method
cpg	270.28	J/mol×K	659.47	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.20	K	1.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.34226e+01
Coeff. B	-3.56060e+03
Coeff. C	-6.21630e+01
Temperature range (K), min.	333.24
Temperature range (K), max.	501.14

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=C2026484&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume