1-Amino-2-butanol

Other names: 2-Butanol, 1-amino-
Inchi: InChI=1S/C4H11NO/c1-2-4(6)3-5/h4,6H,2-3,5H2,1H3
InchiKey: KODLUXHSIZOKTG-UHFFFAOYSA-N
Formula: C4H11NO
SMILES: CCC(O)CN
Mol. weight [g/mol]: 89.14
CAS: 13552-21-1

Physical Properties

Property code	Value	Unit	Source
gf	-90.01	kJ/mol	Joback Method
hf	-249.61	kJ/mol	Joback Method
hfus	11.88	kJ/mol	Joback Method
hvap	51.43	kJ/mol	Joback Method
log10ws	-0.31		Crippen Method
logp	-0.284		Crippen Method
mcvol	83.070	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
tb	442.00	K	NIST Webbook
tc	634.79	K	Joback Method
tf	263.92	K	Joback Method
vc	0.301	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	179.64	J/mol×K	455.19	Joback Method
cpg	187.68	J/mol×K	485.12	Joback Method
cpg	195.38	J/mol×K	515.06	Joback Method
cpg	202.76	J/mol×K	544.99	Joback Method
cpg	209.81	J/mol×K	574.92	Joback Method
cpg	216.56	J/mol×K	604.85	Joback Method
cpg	223.00	J/mol×K	634.79	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61240e+01
Coeff. B	-4.34866e+03
Coeff. C	-6.40400e+01
Temperature range (K), min.	338.64
Temperature range (K), max.	466.23

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=C13552211&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
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume