1-Amino-2-methylbutane

Other names:	2-Methyl-1-butylamine
	2-Methylbutanamine
	2-Methylbutylamine
	Butylamine, 2-methyl-
Inchi:	InChI=1S/C5H13N/c1-3-5(2)4-6/h5H,3-4,6H2,1-2H3
InchiKey:	VJROPLWGFCORRM-UHFFFAOYSA-N
Formula:	C5H13N
SMILES:	CCC(C)CN
Mol. weight [g/mol]:	87.17
CAS:	96-15-1

Physical Properties

Property code	Value	Unit	Source
af	0.3766		Cheméo Relay (1.0)
gf	55.23	kJ/mol	Joback Method
hf	-149.43	kJ/mol	Cheméo Relay (1.0)
hfus	10.38	kJ/mol	Joback Method
hvap	36.19	kJ/mol	Cheméo Relay (1.0)
ie	8.42	eV	Cheméo Relay (1.0)
log10ws	-0.82		Cheméo Relay (1.0)
logp	0.991		Crippen Method
mcvol	91.290	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	701.00		NIST Webbook
tb	368.70	K	NIST Webbook
tb	369.65 ± 2.00	K	NIST Webbook
tb	368.90 ± 2.00	K	NIST Webbook
tc	541.57	K	Cheméo Relay (1.0)
tf	203.50	K	Cheméo Relay (1.0)
vc	0.310	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	173.57	J/mol×K	385.89	Joback Method
cpg	184.03	J/mol×K	416.77	Joback Method
cpg	194.06	J/mol×K	447.66	Joback Method
cpg	203.68	J/mol×K	478.54	Joback Method
cpg	212.89	J/mol×K	509.43	Joback Method
cpg	221.72	J/mol×K	540.31	Joback Method
cpg	230.17	J/mol×K	571.20	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40129e+01
Coeff. B	-2.66199e+03
Coeff. C	-8.53450e+01
Temperature range (K), min.	279.29
Temperature range (K), max.	391.27

Sources

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C96151&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

af: Acentric Factor

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
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