

1-Butanamine, 2-methyl-

Other names:	1-Amino-2-methylbutane 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]:	87.16
CAS:	96-15-1

Physical Properties

Property code	Value	Unit	Source
gf	55.23	kJ/mol	Joback Method
hf	-118.02	kJ/mol	Joback Method
hfus	10.38	kJ/mol	Joback Method
hvap	36.98	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	0.991		Crippen Method
mcpol	91.290	ml/mol	McGowan Method
pc	3749.97	kPa	Joback Method
rinpol	701.00		NIST Webbook
tb	368.90 ± 2.00	K	NIST Webbook
tb	369.65 ± 2.00	K	NIST Webbook
tb	368.70	K	NIST Webbook
tc	571.20	K	Joback Method
tf	214.37	K	Joback Method
vc	0.339	m ³ /kmol	Joback Method

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	$\ln(P_{vp}) = A + B/(T + C)$
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

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=C96151&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/ci9903071

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/30-416-6/1-Butanamine-2-methyl.pdf>

Generated by Cheméo on 2024-04-19 19:44:12.081308462 +0000 UTC m=+15845101.001885779.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.