

1-Butanamine, N-ethyl-

Other names:	Butylamine, N-ethyl- Butylethylamine Ethyl-n-butylamine Ethylbutylamine N-Butyl-N-ethylamine N-Butylethylamine N-Ethyl-n-butylamine N-Ethyl-normal-butylamine N-Ethylbutanamine N-Ethylbutylamine N-n-Butylethylamine
Inchi:	InChI=1S/C6H15N/c1-3-5-6-7-4-2/h7H,3-6H2,1-2H3
InchiKey:	QHCCDDQKNUYGNC-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CCCCNCC
Mol. weight [g/mol]:	101.19
CAS:	13360-63-9

Physical Properties

Property code	Value	Unit	Source
gf	89.03	kJ/mol	Joback Method
hf	-113.70	kJ/mol	Joback Method
hfus	16.39	kJ/mol	Joback Method
hvap	41.40	kJ/mol	NIST Webbook
hvap	40.20 ± 0.10	kJ/mol	NIST Webbook
hvap	40.19	kJ/mol	NIST Webbook
log10ws	-1.52		Crippen Method
logp	1.396		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3152.62	kPa	Joback Method
rinpola	753.00		NIST Webbook
rinpola	744.00		NIST Webbook
rinpola	753.00		NIST Webbook
tb	386.85	K	Joback Method
tc	547.10	K	NIST Webbook
tf	194.95	K	NIST Webbook
vc	0.406	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.47	J/mol×K	556.73	Joback Method
cpg	210.62	J/mol×K	415.16	Joback Method
cpg	221.60	J/mol×K	443.48	Joback Method
cpg	232.16	J/mol×K	471.79	Joback Method
cpg	242.32	J/mol×K	500.10	Joback Method
cpg	252.08	J/mol×K	528.41	Joback Method
cpg	199.23	J/mol×K	386.85	Joback Method
hvapt	33.97	kJ/mol	380.60	NIST Webbook
hvapt	39.10 ± 0.10	kJ/mol	313.00	NIST Webbook
hvapt	38.00 ± 0.10	kJ/mol	328.00	NIST Webbook
hvapt	36.90 ± 0.10	kJ/mol	343.00	NIST Webbook
hvapt	35.80 ± 0.10	kJ/mol	358.00	NIST Webbook
hvapt	39.90	kJ/mol	344.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40218e+01
Coeff. B	-2.77900e+03
Coeff. C	-8.64710e+01
Temperature range (K), min.	288.81
Temperature range (K), max.	405.52

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=C13360639&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.cheméo.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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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