

1-BUTANAMINE, N-ETHYL-N-METHYL-

Inchi: InChI=1S/C7H17N/c1-4-6-7-8(3)5-2/h4-7H2,1-3H3
InchiKey: WOLFCKKMHUVEPN-UHFFFAOYSA-N
Formula: C7H17N
SMILES: CCCCN(C)CC
Mol. weight [g/mol]: 115.22

Physical Properties

Property code	Value	Unit	Source
hfus	16.91	kJ/mol	Joback Method
hvap	37.09	kJ/mol	Cheméo Relay (1.0)
ie	7.83	eV	Cheméo Relay (1.0)
log10ws	-0.74		Cheméo Relay (1.0)
logp	1.738		Crippen Method
mcvol	119.470	ml/mol	McGowan Method
pc	2793.56	kPa	Joback Method
tb	387.11	K	Cheméo Relay (1.0)
tc	546.17	K	Cheméo Relay (1.0)
tf	156.25	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	221.39	J/mol×K	372.00	Joback Method
cpg	234.38	J/mol×K	399.09	Joback Method
cpg	246.88	J/mol×K	426.18	Joback Method
cpg	258.89	J/mol×K	453.28	Joback Method
cpg	270.43	J/mol×K	480.37	Joback Method
cpg	281.51	J/mol×K	507.46	Joback Method
cpg	292.14	J/mol×K	534.55	Joback Method

Sources

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):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C66225409&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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