1-Butanamine, N,N-diethyl-

Other names:	Butylamine, N,N-diethyl- Ethanamine, N-butyl-N-ethyl- N,N-Diethylbutylamine N,N-Diethyl-1-butanamine Diethyl n-butylamine Butyl diethyl amine
Inchi:	InChI=1S/C8H19N/c1-4-7-8-9(5-2)6-3/h4-8H2,1-3H3
InchiKey:	ORSUTASIQKBEFU-UHFFFAOYSA-N
Formula:	C8H19N
SMILES:	CCCCN(CC)CC
Mol. weight [g/mol]:	129.24
CAS:	4444-68-2

Physical Properties

Property code	Value	Unit	Source
gf	127.26	kJ/mol	Joback Method
hf	-140.92	kJ/mol	Joback Method
hfus	19.50	kJ/mol	Joback Method
hvap	35.45	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	2.128		Crippen Method
mcvol	133.560	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
rinpol	838.30		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	838.30		NIST Webbook
rinpol	854.00		NIST Webbook
rinpol	846.00		NIST Webbook
rinpol	846.00		NIST Webbook
tb	409.15 ± 3.00	K	NIST Webbook
tc	557.19	K	Joback Method
tf	212.39	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.25	J/mol×K	394.88	Joback Method
cpg	275.33	J/mol×K	421.93	Joback Method
cpg	288.87	J/mol×K	448.98	Joback Method
cpg	301.88	J/mol×K	476.04	Joback Method
cpg	314.38	J/mol×K	503.09	Joback Method
cpg	326.38	J/mol×K	530.14	Joback Method
cpg	337.90	J/mol×K	557.19	Joback Method

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=C4444682&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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