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]:	129.25

Physical Properties

Property code	Value	Unit	Source
af	0.4011		Cheméo Relay (1.0)
gf	127.26	kJ/mol	Joback Method
hf	-148.82	kJ/mol	Cheméo Relay (1.0)
hfus	19.50	kJ/mol	Joback Method
hvap	43.37	kJ/mol	Cheméo Relay (1.0)
ie	7.70	eV	Cheméo Relay (1.0)
log10ws	-1.19		Cheméo Relay (1.0)
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	574.03	K	Cheméo Relay (1.0)
tf	168.47	K	Cheméo Relay (1.0)
vc	0.500	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	-1.50750e+01
Coeff. B	8.87760e-01
Coeff. C	-5.24000e-04
Coeff. D	1.21400e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

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=C4444682&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

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