

1-Butanamine, N-butyl-N-methyl-

Other names: Dibutylamine, N-methyl-
Dibutylmethylanine
Methanamine, N,N-dibutyl-
Methyl di-n-butylamine
Methyldibutylamine
N,N-Dibutyl-N-methylamine
N,N-Dibutylmethylanine
N,N-di-n-Butylmethylanine
N-Butyl-N-methyl-1-butanamine
N-Methyldibutylamine
di-n-Butylmethylanine

Inchi: InChI=1S/C9H21N/c1-4-6-8-10(3)9-7-5-2/h4-9H2,1-3H3

InchiKey: MTHFROHDIWGWFD-UHFFFAOYSA-N

Formula: C9H21N

SMILES: CCCCCN(C)CCCC

Mol. weight [g/mol]: 143.27

CAS: 3405-45-6

Physical Properties

Property code	Value	Unit	Source
gf	135.68	kJ/mol	Joback Method
hf	-161.56	kJ/mol	Joback Method
hfus	22.09	kJ/mol	Joback Method
hvap	37.67	kJ/mol	Joback Method
log10ws	-2.16		Crippen Method
logp	2.518		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
rinpol	923.60		NIST Webbook
rinpol	948.00		NIST Webbook
tb	417.76	K	Joback Method
tc	579.60	K	Joback Method
tf	223.66	K	Joback Method
vc	0.557	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.35	J/molxK	417.76	Joback Method
cpg	318.41	J/molxK	444.73	Joback Method
cpg	332.88	J/molxK	471.71	Joback Method
cpg	346.79	J/molxK	498.68	Joback Method
cpg	360.15	J/molxK	525.66	Joback Method
cpg	372.97	J/molxK	552.63	Joback Method
cpg	385.27	J/molxK	579.60	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	323.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.54791e+01
Coeff. B	-4.05227e+03
Coeff. C	-6.14540e+01
Temperature range (K), min.	328.20
Temperature range (K), max.	460.00

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=C3405456&Units=SI

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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