

# 1-Butanamine, 3-methyl, N,N-diethyl

<b>Other names:</b>	Diethyl isoamylamine
<b>Inchi:</b>	InChI=1S/C9H21N/c1-5-10(6-2)8-7-9(3)4/h9H,5-8H2,1-4H3
<b>InchiKey:</b>	FJPUTKPSUZLWMN-UHFFFAOYSA-N
<b>Formula:</b>	C9H21N
<b>SMILES:</b>	CCN(CC)CCC(C)C
<b>Mol. weight [g/mol]:</b>	143.27

## Physical Properties

Property code	Value	Unit	Source
gf	133.24	kJ/mol	Joback Method
hf	-166.84	kJ/mol	Joback Method
hfus	18.56	kJ/mol	Joback Method
hvap	37.28	kJ/mol	Joback Method
log10ws	-1.92		Crippen Method
logp	2.374		Crippen Method
mcvol	147.650	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
rinpol	902.00		NIST Webbook
rinpol	902.00		NIST Webbook
tb	417.32	K	Joback Method
tc	582.69	K	Joback Method
tf	208.66	K	Joback Method
vc	0.551	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.29	J/mol×K	417.32	Joback Method
cpg	318.76	J/mol×K	444.88	Joback Method
cpg	333.62	J/mol×K	472.44	Joback Method
cpg	347.88	J/mol×K	500.01	Joback Method
cpg	361.56	J/mol×K	527.57	Joback Method
cpg	374.67	J/mol×K	555.13	Joback Method
cpg	387.23	J/mol×K	582.69	Joback Method

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R12832&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R12832&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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