

1-Butanamine, N,3-dimethyl-

Other names:	Butylamine, N,3-dimethyl- N-Methylisoamylamine N-Methylisopentylamine Methyl isopentyl amine isoamylmethyl-amine
Inchi:	InChI=1S/C6H15N/c1-6(2)4-5-7-3/h6-7H,4-5H2,1-3H3
InchiKey:	QSOCODZVGPDGDA-UHFFFAOYSA-N
Formula:	C6H15N
SMILES:	CNCCC(C)C
Mol. weight [g/mol]:	101.19
CAS:	4104-44-3

Physical Properties

Property code	Value	Unit	Source
gf	86.59	kJ/mol	Joback Method
hf	-118.98	kJ/mol	Joback Method
hfus	12.87	kJ/mol	Joback Method
hvap	35.00	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.252		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3181.14	kPa	Joback Method
rinpol	751.00		NIST Webbook
rinpol	751.00		NIST Webbook
tb	382.15 ± 3.00	K	NIST Webbook
tb	381.15 ± 4.00	K	NIST Webbook
tb	368.15 ± 3.00	K	NIST Webbook
tc	560.25	K	Joback Method
tf	195.04	K	Joback Method
vc	0.401	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	199.15	J/mol×K	386.41	Joback Method
cpg	210.90	J/mol×K	415.38	Joback Method
cpg	222.20	J/mol×K	444.36	Joback Method
cpg	233.07	J/mol×K	473.33	Joback Method
cpg	243.51	J/mol×K	502.30	Joback Method
cpg	253.53	J/mol×K	531.27	Joback Method
cpg	263.15	J/mol×K	560.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4104443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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