

# 1-Butanamine, 3-methyl-N,N-bis(3-methylbutyl)-

<b>Other names:</b>	Tri(3-methylbutyl)amine Triisoamylamine Triisopentylamine Tris(3-methylbutyl)amine
<b>Inchi:</b>	InChI=1S/C15H33N/c1-13(2)7-10-16(11-8-14(3)4)12-9-15(5)6/h13-15H,7-12H2,1-6H3
<b>InchiKey:</b>	QKVUSSUOYHTOFQ-UHFFFAOYSA-N
<b>Formula:</b>	C15H33N
<b>SMILES:</b>	CC(C)CCN(CCC(C)C)CCC(C)C
<b>Mol. weight [g/mol]:</b>	227.43
<b>CAS:</b>	645-41-0

## Physical Properties

Property code	Value	Unit	Source
chl	-10277.00	kJ/mol	NIST Webbook
gf	178.88	kJ/mol	Joback Method
hf	-301.24	kJ/mol	Joback Method
hfl	-342.00	kJ/mol	NIST Webbook
hfus	27.06	kJ/mol	Joback Method
hvap	49.86	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	4.427		Crippen Method
mcvol	232.190	ml/mol	McGowan Method
pc	1439.16	kPa	Joback Method
tb	553.72	K	Joback Method
tc	719.95	K	Joback Method
tf	246.28	K	Joback Method
vc	0.875	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	597.28	J/molxK	553.72	Joback Method
cpg	617.48	J/molxK	581.43	Joback Method
cpg	636.81	J/molxK	609.13	Joback Method

cpg	655.32	J/mol×K	636.84	Joback Method
cpg	673.01	J/mol×K	664.54	Joback Method
cpg	689.92	J/mol×K	692.25	Joback Method
cpg	706.08	J/mol×K	719.95	Joback Method

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.32383e+01
Coeff. B	-3.96426e+03
Coeff. C	-8.24160e+01
Temperature range (K), min.	388.52
Temperature range (K), max.	582.52

## Sources

<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<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=C645410&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C645410&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<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>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</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>pvap:</b>	Vapor pressure
<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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