

# 3-Butoxypropylamine

<b>Other names:</b>	1-Propanamine, 3-butoxy- 3-Butoxypropanamine 3-aminopropyl butyl ether 3-butoxy-1-propanamine 3-n-Butoxy-1-propylamine
<b>Inchi:</b>	InChI=1S/C7H17NO/c1-2-3-6-9-7-4-5-8/h2-8H2,1H3
<b>InchiKey:</b>	LPUBRQWGZPPVBS-UHFFFAOYSA-N
<b>Formula:</b>	C7H17NO
<b>SMILES:</b>	CCCCOCCN
<b>Mol. weight [g/mol]:</b>	131.22
<b>CAS:</b>	16499-88-0

## Physical Properties

Property code	Value	Unit	Source
gf	-30.49	kJ/mol	Joback Method
hf	-286.24	kJ/mol	Joback Method
hfus	20.27	kJ/mol	Joback Method
hvap	44.23	kJ/mol	Joback Method
log10ws	-1.27		Crippen Method
logp	1.152		Crippen Method
mcvol	125.340	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
tb	454.51	K	Joback Method
tc	632.78	K	Joback Method
tf	274.14	K	Joback Method
vc	0.474	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.78	J/mol×K	454.51	Joback Method
cpg	287.10	J/mol×K	484.22	Joback Method
cpg	298.98	J/mol×K	513.93	Joback Method
cpg	310.43	J/mol×K	543.65	Joback Method

cpg	321.44	J/mol×K	573.36	Joback Method
cpg	332.03	J/mol×K	603.07	Joback Method
cpg	342.20	J/mol×K	632.78	Joback Method
rh <sub>ol</sub>	855.84	kg/m <sup>3</sup>	283.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K
rh <sub>ol</sub>	851.46	kg/m <sup>3</sup>	288.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K
rh <sub>ol</sub>	847.07	kg/m <sup>3</sup>	293.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K
rh <sub>ol</sub>	842.68	kg/m <sup>3</sup>	298.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K
rh <sub>ol</sub>	838.29	kg/m <sup>3</sup>	303.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
t <sub>brp</sub>	442.70	K	101.00	NIST Webbook

## Correlations

Information	Value
Property code	p <sub>vap</sub>
Equation	$\ln(P_{vap}) = A + B/(T + C)$
Coeff. A	1.65105e+01
Coeff. B	-4.48952e+03

Coeff. C	-6.51800e+01
Temperature range (K), min.	341.92
Temperature range (K), max.	466.07

## Sources

<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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures Between 283 K and 315 K:</b>	<a href="https://www.doi.org/10.1021/acs.jced.7b00006">https://www.doi.org/10.1021/acs.jced.7b00006</a>
<b>3-Ethoxypropan-1-amine and 3-Butoxypropan-1-amine in Water at 298.15 K:</b>	<a href="https://www.doi.org/10.1021/acs.jced.7b00900">https://www.doi.org/10.1021/acs.jced.7b00900</a>
<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=C16499880&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16499880&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>

## 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>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>rhol:</b>	Liquid Density
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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