3-BUTOXYPROPYLAMINE

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

Physical Properties

Property code	Value	Unit	Source
af	0.5589		Cheméo Relay (1.0)
gf	-30.49	kJ/mol	Joback Method
hf	-304.26	kJ/mol	Cheméo Relay (1.0)
hfus	20.27	kJ/mol	Joback Method
hvap	47.18	kJ/mol	Cheméo Relay (1.0)
ie	8.97	eV	Cheméo Relay (1.0)
log10ws	-0.64		Cheméo Relay (1.0)
logp	1.152		Crippen Method
mcvol	125.340	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
tb	446.93	K	Cheméo Relay (1.0)
tc	622.21	K	Cheméo Relay (1.0)
tf	216.81	K	Cheméo Relay (1.0)
vc	0.459	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.78	J/mol×K	454.51	Joback Method
cpg	342.20	J/mol×K	632.78	Joback Method

cpg	332.03	J/mol×K	603.07	Joback Method
cpg	321.44	J/mol×K	573.36	Joback Method
cpg	310.43	J/mol×K	543.65	Joback Method
cpg	298.98	J/mol×K	513.93	Joback Method
cpg	287.10	J/mol×K	484.22	Joback Method
rhol	842.68	kg/m3	298.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K
rhol	838.29	kg/m3	303.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K
rhol	847.07	kg/m3	293.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K
rhol	851.46	kg/m3	288.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K
rhol	855.84	kg/m3	283.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K
speedsl	1387.33	m/s	283.15	Ultrasound speeds and molar isentropic compressions of (3-butoxypropan-1-amine + water) mixtures from T = (283.15 to 303.15) K
speedsl	1306.74	m/s	303.15	Ultrasound speeds and molar isentropic compressions of (3-butoxypropan-1-amine + water) mixtures from T = (283.15 to 303.15) K
speedsl	1326.39	m/s	298.15	Ultrasound speeds and molar isentropic compressions of (3-butoxypropan-1-amine + water) mixtures from T = (283.15 to 303.15) K

speedsl	1346.70	m/s	293.15	Ultrasound speeds and molar isentropic compressions of (3-butoxypropan-1-amine + water) mixtures from T = (283.15 to 303.15) K
speedsl	1367.30	m/s	288.15	Ultrasound speeds and molar isentropic compressions of (3-butoxypropan-1-amine + water) mixtures from T = (283.15 to 303.15) K

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	442.70	K	101.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = 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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0, beta):

A volumetric and acoustic study of pseudo-binary mixtures of (water + 1,3 propanediol + 3-Butoxypropan-1-amine) from T = (283.15 to 303.15) K:	https://www.doi.org/10.1016/j.jct.2018.08.033
Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K:	https://www.doi.org/10.1021/acs.jced.7b00006
NIST WebBook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16499880&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Ultrasound speeds and molar isentropic compressions of (3-butoxypropan-1-amine + water) mixtures from T = (283.15 to 303.15) K:	https://www.doi.org/10.1016/j.jct.2017.05.010
Excess Partial Molar Enthalpies of 3-Ethoxypropan-1-amine and 3-Butoxypropan-1-amine in Water at 298.15 K:	https://www.doi.org/10.1021/acs.jced.7b00900

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
speedsl:	Speed of sound in fluid
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume