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
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
rhol	855.84	kg/m3	283.15	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	847.07	kg/m3	293.15	Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 303.15 K
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

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16499880&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Volumetric Study of 3-Butoxypropan-1-amine + Water Mixtures between 283.15 and 353.15 K:	https://www.doi.org/10.1021/acs.jced.7b00006
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
pvap:	Vapor pressure
rhol:	Liquid Density
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume