3-butoxy-1-propanol

Inchi: InChI=1S/C7H16O2/c1-2-3-6-9-7-4-5-8/h8H,2-7H2,1H3
InchiKey: NTKBNCABAMQDIG-UHFFFAOYSA-N
Formula: C7H16O2
SMILES: CCCCOCCCO
Mol. weight [g/mol]: 132.20
CAS: 10215-33-5

Physical Properties

Property code	Value	Unit	Source
af	0.7077		Cheméo Relay (1.0)
gf	-233.76	kJ/mol	Joback Method
hf	-482.07	kJ/mol	Cheméo Relay (1.0)
hfus	19.16	kJ/mol	Joback Method
hvap	66.06	kJ/mol	Cheméo Relay (1.0)
ie	9.62	eV	Cheméo Relay (1.0)
log10ws	-0.58		Cheméo Relay (1.0)
logp	1.185		Crippen Method
mcvol	121.230	ml/mol	McGowan Method
pc	3035.62	kPa	Joback Method
tb	465.60	K	Cheméo Relay (1.0)
tc	647.31	K	Cheméo Relay (1.0)
tf	217.61	K	Cheméo Relay (1.0)
vc	0.452	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	271.34	J/mol×K	474.16	Joback Method
cpg	281.77	J/mol×K	500.92	Joback Method
cpg	291.85	J/mol×K	527.67	Joback Method
cpg	301.60	J/mol×K	554.43	Joback Method
cpg	311.01	J/mol×K	581.19	Joback Method
cpg	320.10	J/mol×K	607.95	Joback Method
cpg	328.87	J/mol×K	634.70	Joback Method

dvisc	0.0300573	Pa×s	251.70	Joback Method
dvisc	0.0071642	Pa×s	288.78	Joback Method
dvisc	0.0023665	Pa×s	325.85	Joback Method
dvisc	0.0009802	Pa×s	362.93	Joback Method
dvisc	0.0004781	Pa×s	400.01	Joback Method
dvisc	0.0002634	Pa×s	437.08	Joback Method
dvisc	0.0001593	Pa×s	474.16	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.20955e+01
Coeff. B	-6.55365e+03
Coeff. C	-7.73100e+01
Temperature range (K), min.	377.83
Temperature range (K), max.	467.78

Sources

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

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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume