

2-Propanol, 1-chloro-3-butoxy

Inchi:	InChI=1S/C7H15ClO2/c1-2-3-4-10-6-7(9)5-8/h7,9H,2-6H2,1H3
InchiKey:	IZHGMMBZJWHGND-UHFFFAOYSA-N
Formula:	C7H15ClO2
SMILES:	CCCCOCC(O)CCl
Mol. weight [g/mol]:	166.65

Physical Properties

Property code	Value	Unit	Source
gf	-248.13	kJ/mol	Joback Method
hf	-493.28	kJ/mol	Joback Method
hfus	19.84	kJ/mol	Joback Method
hvap	54.26	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.403		Crippen Method
mcvol	133.470	ml/mol	McGowan Method
pc	2940.89	kPa	Joback Method
rinsol	1150.00		NIST Webbook
tb	511.15	K	Joback Method
tc	680.43	K	Joback Method
tf	266.62	K	Joback Method
vc	0.507	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.33	J/molxK	511.15	Joback Method
cpg	308.67	J/molxK	539.36	Joback Method
cpg	318.63	J/molxK	567.58	Joback Method
cpg	328.21	J/molxK	595.79	Joback Method
cpg	337.41	J/molxK	624.00	Joback Method
cpg	346.24	J/molxK	652.21	Joback Method
cpg	354.70	J/molxK	680.43	Joback Method
dvisc	0.0289638	Paxs	266.62	Joback Method
dvisc	0.0064495	Paxs	307.38	Joback Method

dvisc	0.0020414	Paxs	348.13	Joback Method
dvisc	0.0008223	Paxs	388.88	Joback Method
dvisc	0.0003936	Paxs	429.64	Joback Method
dvisc	0.0002141	Paxs	470.39	Joback Method
dvisc	0.0001283	Paxs	511.15	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313901&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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