2-Propanol, 1-chloro-3-isobutoxy

Inchi: InChI=1S/C7H15ClO2/c1-6(2)4-10-5-7(9)3-8/h6-7,9H,3-5H2,1-2H3
InchiKey: OYLSNRGLWVHWNI-UHFFFAOYSA-N
Formula: C7H15ClO2
SMILES: CC(C)COCC(O)CCl
Mol. weight [g/mol]: 166.65

Physical Properties

Property code	Value	Unit	Source
gf	-250.57	kJ/mol	Joback Method
hf	-498.56	kJ/mol	Joback Method
hfus	16.31	kJ/mol	Joback Method
hvap	53.87	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.259		Crippen Method
mcvol	133.470	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1130.00		NIST Webbook
rinpol	1130.00		NIST Webbook
tb	510.71	K	Joback Method
tc	683.29	K	Joback Method
tf	251.62	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.61	J/mol×K	510.71	Joback Method
cpg	309.22	J/mol×K	539.47	Joback Method
cpg	319.42	J/mol×K	568.24	Joback Method
cpg	329.22	J/mol×K	597.00	Joback Method
cpg	338.62	J/mol×K	625.76	Joback Method
cpg	347.63	J/mol×K	654.53	Joback Method
cpg	356.25	J/mol×K	683.29	Joback Method
dvisc	0.0578400	Pa×s	251.62	Joback Method

dvisc	0.0097512	Pa×s	294.80	Joback Method
dvisc	0.0025909	Pa×s	337.98	Joback Method
dvisc	0.0009295	Pa×s	381.16	Joback Method
dvisc	0.0004109	Pa×s	424.35	Joback Method
dvisc	0.0002112	Pa×s	467.53	Joback Method
dvisc	0.0001215	Pa×s	510.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313916&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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