1-chloro-1-propanol

Inchi: InChI=1S/C3H7ClO/c1-2-3(4)5/h3,5H,2H2,1H3
InchiKey: RZWHKKIXMPLQEM-UHFFFAOYSA-N
Formula: C3H7ClO
SMILES: CCC(O)Cl
Mol. weight [g/mol]: 94.54

Physical Properties

Property code	Value	Unit	Source
gf	-176.81	kJ/mol	Joback Method
hf	-278.50	kJ/mol	Joback Method
hfus	8.29	kJ/mol	Joback Method
hvap	42.95	kJ/mol	Joback Method
log10ws	-1.10		Crippen Method
logp	0.954		Crippen Method
mcvol	71.240	ml/mol	McGowan Method
pc	4802.50	kPa	Joback Method
rinpol	678.00		NIST Webbook
rinpol	678.00		NIST Webbook
tb	397.21	K	Joback Method
tc	571.23	K	Joback Method
tf	199.31	K	Joback Method
vc	0.266	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	122.10	J/mol×K	397.21	Joback Method
cpg	148.55	J/mol×K	542.23	Joback Method
cpg	143.70	J/mol×K	513.23	Joback Method
cpg	138.64	J/mol×K	484.22	Joback Method
cpg	133.36	J/mol×K	455.22	Joback Method
cpg	127.85	J/mol×K	426.21	Joback Method
cpg	153.19	J/mol×K	571.23	Joback Method
dvisc	0.0003683	Pa×s	397.21	Joback Method

dvisc	0.0006545	Pa×s	364.23	Joback Method
dvisc	0.0013040	Pa×s	331.24	Joback Method
dvisc	0.0030263	Pa×s	298.26	Joback Method
dvisc	0.0086584	Pa×s	265.28	Joback Method
dvisc	0.0333896	Pa×s	232.29	Joback Method
dvisc	0.2012782	Pa×s	199.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R216236&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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