(S)-(+)-2-Chloro-1-propanol

Other names: (S)-(+)-2-Chloropropan-1-ol
Inchi: InChI=1S/C3H7ClO/c1-3(4)2-5/h3,5H,2H2,1H3/t3-/m1/s1
InchiKey: VZIQXGLTRZLBEX-GSVOUGTGSA-N
Formula: C3H7ClO
SMILES: CC(Cl)CO
Mol. weight [g/mol]: 94.54
CAS: 19210-21-0

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	-0.61		Crippen Method
logp	0.606		Crippen Method
mcvol	71.240	ml/mol	McGowan Method
pc	4802.50	kPa	Joback Method
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	127.85	J/mol×K	426.21	Joback Method
cpg	133.36	J/mol×K	455.22	Joback Method
cpg	138.64	J/mol×K	484.22	Joback Method
cpg	143.70	J/mol×K	513.23	Joback Method
cpg	148.55	J/mol×K	542.23	Joback Method
cpg	153.19	J/mol×K	571.23	Joback Method
dvisc	0.2012782	Pa×s	199.31	Joback Method

dvisc	0.0333896	Pa×s	232.29	Joback Method
dvisc	0.0086584	Pa×s	265.28	Joback Method
dvisc	0.0030263	Pa×s	298.26	Joback Method
dvisc	0.0013040	Pa×s	331.24	Joback Method
dvisc	0.0006545	Pa×s	364.23	Joback Method
dvisc	0.0003683	Pa×s	397.21	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.50	K	10.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C19210210&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume