Propanoic acid, 3-chloro-

Other names:	Propionic acid, 3-chloro-
	«beta»-Chloropropionic acid
	«beta»-Monochloropropionic acid
	3-Chloropropanoic acid
	3-Chloropropionic acid
Inchi:	InChI=1S/C3H5ClO2/c4-2-1-3(5)6/h1-2H2,(H,5,6)
InchiKey:	QEYMMOKECZBKAC-UHFFFAOYSA-N
Formula:	C3H5ClO2
SMILES:	O=C(O)CCCl
Mol. weight [g/mol]:	108.52
CAS:	107-94-8

Physical Properties

Property code	Value	Unit	Source
chs	-1370.00 ± 3.00	kJ/mol	NIST Webbook
chs	-1366.00	kJ/mol	NIST Webbook
gf	-303.29	kJ/mol	Joback Method
hf	-385.80	kJ/mol	Joback Method
hfus	13.41	kJ/mol	Joback Method
hvap	50.08	kJ/mol	Joback Method
log10ws	-0.33		Crippen Method
logp	0.700		Crippen Method
mcvol	72.810	ml/mol	McGowan Method
pc	5190.64	kPa	Joback Method
rinpol	970.00		NIST Webbook
rinpol	960.40		NIST Webbook
tb	477.20	K	NIST Webbook
tc	633.22	K	Joback Method
tf	314.00 ± 4.00	K	NIST Webbook
vc	0.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	130.07	J/mol×K	451.52	Joback Method
cpg	135.03	J/mol×K	481.80	Joback Method
cpg	139.77	J/mol×K	512.09	Joback Method
cpg	144.30	J/mol×K	542.37	Joback Method
cpg	148.61	J/mol×K	572.65	Joback Method
cpg	152.71	J/mol×K	602.93	Joback Method
cpg	156.61	J/mol×K	633.22	Joback Method
dvisc	0.0223163	Pa×s	264.24	Joback Method
dvisc	0.0074920	Pa×s	295.45	Joback Method
dvisc	0.0030985	Pa×s	326.67	Joback Method
dvisc	0.0014949	Pa×s	357.88	Joback Method
dvisc	0.0008107	Pa×s	389.09	Joback Method
dvisc	0.0004814	Pa×s	420.31	Joback Method
dvisc	0.0003073	Pa×s	451.52	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C107948&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

chs: Standard solid enthalpy of combustion
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