Butanoic acid, 2-chloro-

Other names:	Butyric acid, 2-chloro-
	«alpha»-Chlorobutyric acid
	2-Chlorobutyric acid
	2-Chlorobutanoic acid
	«alpha»-Chloro-n-butyric acid
Inchi:	InChI=1S/C4H7ClO2/c1-2-3(5)4(6)7/h3H,2H2,1H3,(H,6,7)
InchiKey:	RVBUZBPJAGZHSQ-UHFFFAOYSA-N
Formula:	C4H7ClO2
SMILES:	CCC(Cl)C(=O)O
Mol. weight [g/mol]:	122.55
CAS:	4170-24-5

Physical Properties

Property code	Value	Unit	Source
chl	-2022.50 ± 8.40	kJ/mol	NIST Webbook
chl	-2018.00	kJ/mol	NIST Webbook
gf	-297.31	kJ/mol	Joback Method
hf	-411.72	kJ/mol	Joback Method
hfus	12.48	kJ/mol	Joback Method
hvap	51.92	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	1.088		Crippen Method
mcvol	86.900	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
tb	473.96	K	Joback Method
tc	657.92	K	Joback Method
tf	260.51	K	Joback Method
vc	0.328	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.29	J/mol×K	473.96	Joback Method
cpg	196.72	J/mol×K	627.26	Joback Method

cpg	191.41	J/mol×K	596.60	Joback Method
cpg	185.81	J/mol×K	565.94	Joback Method
cpg	179.93	J/mol×K	535.28	Joback Method
cpg	173.76	J/mol×K	504.62	Joback Method
cpg	201.77	J/mol×K	657.92	Joback Method
dvisc	0.0002468	Pa×s	473.96	Joback Method
dvisc	0.0004028	Pa×s	438.38	Joback Method
dvisc	0.0007170	Pa×s	402.81	Joback Method
dvisc	0.0014271	Pa×s	367.24	Joback Method
dvisc	0.0032924	Pa×s	331.66	Joback Method
dvisc	0.0092852	Pa×s	296.08	Joback Method
dvisc	0.0347585	Pa×s	260.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4170245&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

chl:	Standard liquid 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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