Butanoic acid, 4-chloro-

Other names:	Butyric acid, 4-chloro-
	«gamma»-Chlorobutyric acid
	Gammachlorobutyric acid
	4-Chlorobutanoic acid
	4-Chlorobutyric acid
	Cl(CH2)3COOH
	«gamma»-Chloro-n-butyric acid
Inchi:	InChI=1S/C4H7ClO2/c5-3-1-2-4(6)7/h1-3H2,(H,6,7)
InchiKey:	IPLKGJHGWCVSOG-UHFFFAOYSA-N
Formula:	C4H7ClO2
SMILES:	O=C(O)CCCCl
Mol. weight [g/mol]:	122.55
CAS:	627-00-9

Physical Properties

Property code	Value	Unit	Source
chl	-2031.80 ± 8.40	kJ/mol	NIST Webbook
chl	-2028.00	kJ/mol	NIST Webbook
gf	-294.87	kJ/mol	Joback Method
hf	-406.44	kJ/mol	Joback Method
hfus	16.00	kJ/mol	Joback Method
hvap	52.31	kJ/mol	Joback Method
log10ws	-0.75		Crippen Method
logp	1.090		Crippen Method
mcvol	86.900	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
rinpol	1063.10		NIST Webbook
tb	474.40	K	Joback Method
tc	654.46	K	Joback Method
tf	275.51	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.03	J/mol×K	474.40	Joback Method
cpg	173.29	J/mol×K	504.41	Joback Method
cpg	179.27	J/mol×K	534.42	Joback Method
cpg	184.98	J/mol×K	564.43	Joback Method
cpg	190.42	J/mol×K	594.44	Joback Method
cpg	195.60	J/mol×K	624.45	Joback Method
cpg	200.53	J/mol×K	654.46	Joback Method
dvisc	0.0190491	Pa×s	275.51	Joback Method
dvisc	0.0063353	Pa×s	308.66	Joback Method
dvisc	0.0026085	Pa×s	341.81	Joback Method
dvisc	0.0012565	Pa×s	374.95	Joback Method
dvisc	0.0006815	Pa×s	408.10	Joback Method
dvisc	0.0004052	Pa×s	441.25	Joback Method
dvisc	0.0002591	Pa×s	474.40	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	469.20	K	2.90	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C627009&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume