Butanoic acid, 4-chloro-, methyl ester

Other names:	4-Chlorobutanoic acid methyl ester
	4-Chlorobutyric acid methyl ester
	Butyric acid, 4-chloro-, methyl ester
	ClCH2(CH2)2C(O)OCH3
	Methyl «gamma»-chlorobutyrate
	Methyl «omega»-chlorobutyrate
	methyl 4-chlorobutanoate
	methyl 4-chlorobutyrate
	«gamma»-Chlorobutyric acid methyl ester
Inchi:	InChI=1S/C5H9ClO2/c1-8-5(7)3-2-4-6/h2-4H2,1H3
InchiKey:	ZZUYIRISBMWFMV-UHFFFAOYSA-N
Formula:	C5H9ClO2
SMILES:	COC(=O)CCCCl
Mol. weight [g/mol]:	136.58
CAS:	3153-37-5

Physical Properties

Property code	Value	Unit	Source
chl	-2733.00	kJ/mol	NIST Webbook
gf	-254.63	kJ/mol	Joback Method
hf	-407.07	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	40.27	kJ/mol	Joback Method
ie	10.30 ± 0.30	eV	NIST Webbook
log10ws	-0.93		Crippen Method
logp	1.178		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
rinpol	972.20		NIST Webbook
rinpol	927.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	972.20		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	933.00		NIST Webbook

rinpol	920.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	941.00		NIST Webbook
tb	448.70	K	NIST Webbook
tc	613.54	K	Joback Method
tf	248.19	K	Joback Method
vc	0.389	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.82	J/mol×K	427.52	Joback Method
cpg	195.11	J/mol×K	458.52	Joback Method
cpg	203.12	J/mol×K	489.53	Joback Method
cpg	210.84	J/mol×K	520.53	Joback Method
cpg	218.28	J/mol×K	551.53	Joback Method
cpg	225.43	J/mol×K	582.53	Joback Method
cpg	232.29	J/mol×K	613.54	Joback Method
dvisc	0.0015190	Pa×s	298.15	Densities and Viscosities of Binary Mixtures of Methyl 4-Chlorobutyrate with Aromatic Hydrocarbons at T) (298.15 to 318.15) K
dvisc	0.0012790	Pa×s	308.15	Densities and Viscosities of Binary Mixtures of Methyl 4-Chlorobutyrate with Aromatic Hydrocarbons at T) (298.15 to 318.15) K
dvisc	0.0010890	Pa×s	318.15	Densities and Viscosities of Binary Mixtures of Methyl 4-Chlorobutyrate with Aromatic Hydrocarbons at T) (298.15 to 318.15) K

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Densities and Viscosities of Binary Mixtures of Methyl 4-Chlorobutyrate with Aromatic Hydrocarbons at T) (298.15 to 318.15) K:	https://www.doi.org/10.1021/je900194v
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3153375&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie:	Ionization energy
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