ETHYL 4-CHLOROBUTYRATE

Other names:	Butyric acid, 4-chloro-, ethyl ester
	Ethyl «gamma»-chlorobutyrate
	Ethyl 4-chlorobutanoate
	Ethyl 4-chlorobutyrate
	4-Chlorobutanoic acid ethyl ester
	Cl(CH2)3C(O)OC2H5
	«gamma»-Chlorobutyric acid ethyl ester
	Ethyl «omega»-chlorobutyrate
	4-Chlorobutyric acid ethyl ester
	NSC 81215
Inchi:	InChI=1S/C6H11ClO2/c1-2-9-6(8)4-3-5-7/h2-5H2,1H3
InchiKey:	OPXNFHAILOHHFO-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CCOC(=O)CCCCl
Mol. weight [g/mol]:	150.61

Physical Properties

Property code	Value	Unit	Source
af	0.4799		Cheméo Relay (1.0)
chl	-3383.00	kJ/mol	NIST Webbook
chl	-3390.30 ± 8.40	kJ/mol	NIST Webbook
gf	-246.21	kJ/mol	Joback Method
hf	-513.80 ± 9.60	kJ/mol	NIST Webbook
hfl	-566.50 ± 8.40	kJ/mol	NIST Webbook
hfus	18.28	kJ/mol	Joback Method
hvap	52.70 ± 4.20	kJ/mol	NIST Webbook
ie	10.16	eV	Cheméo Relay (1.0)
log10ws	-1.40		Cheméo Relay (1.0)
logp	1.569		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
rinpol	1002.00		NIST Webbook
rinpol	1018.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1022.00		NIST Webbook
tb	459.20	K	NIST Webbook

tc	633.75	K	Cheméo Relay (1.0)
tf	211.78	K	Cheméo Relay (1.0)
vc	0.424	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	224.90	J/mol×K	450.40	Joback Method
cpg	234.51	J/mol×K	481.13	Joback Method
cpg	243.77	J/mol×K	511.86	Joback Method
cpg	252.68	J/mol×K	542.58	Joback Method
cpg	261.25	J/mol×K	573.31	Joback Method
cpg	269.47	J/mol×K	604.04	Joback Method
cpg	277.34	J/mol×K	634.77	Joback Method
dvisc	0.0030315	Pa×s	259.46	Joback Method
dvisc	0.0016707	Pa×s	291.28	Joback Method
dvisc	0.0010354	Pa×s	323.11	Joback Method
dvisc	0.0006992	Pa×s	354.93	Joback Method
dvisc	0.0005036	Pa×s	386.75	Joback Method
dvisc	0.0003813	Pa×s	418.58	Joback Method
dvisc	0.0003003	Pa×s	450.40	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3153364&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af: Acentric Factor
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
hfl:	Liquid phase 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