Ethyl 2-chlorobutanoate

Other names:	Ethanol, 2-chloro, butanoate
	Butanoic acid, 2-chloroethyl ester
	Ethyl 2-chlorobutanoate
	Ethyl 2-chlorobutyrate
Inchi:	InChI=1S/C6H11ClO2/c1-3-5(7)6(8)9-4-2/h5H,3-4H2,1-2H3
InchiKey:	QTEITWPJVHAOTN-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CCOC(=O)C(Cl)CC
Mol. weight [g/mol]:	150.61

Physical Properties

Property code	Value	Unit	Source
af	0.4102		Cheméo Relay (1.0)
chl	-3338.00	kJ/mol	NIST Webbook
gf	-248.65	kJ/mol	Joback Method
hf	-541.33	kJ/mol	Cheméo Relay (1.0)
hfus	14.76	kJ/mol	Joback Method
hvap	47.37	kJ/mol	Cheméo Relay (1.0)
ie	10.10	eV	Cheméo Relay (1.0)
log10ws	-1.72		Cheméo Relay (1.0)
logp	1.567		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	976.00		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	945.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	945.00		NIST Webbook
ripol	1510.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1493.00		NIST Webbook
ripol	1473.00		NIST Webbook

ripol	1510.00		NIST Webbook
tb	417.08	K	Cheméo Relay (1.0)
tc	612.72	K	Cheméo Relay (1.0)
tf	229.81	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	225.04	J/mol×K	449.96	Joback Method
cpg	278.93	J/mol×K	638.50	Joback Method
cpg	270.88	J/mol×K	607.08	Joback Method
cpg	262.46	J/mol×K	575.65	Joback Method
cpg	253.66	J/mol×K	544.23	Joback Method
cpg	244.50	J/mol×K	512.81	Joback Method
cpg	234.96	J/mol×K	481.38	Joback Method
dvisc	0.0007450	Pa×s	347.21	Joback Method
dvisc	0.0002866	Pa×s	449.96	Joback Method
dvisc	0.0003739	Pa×s	415.71	Joback Method
dvisc	0.0005117	Pa×s	381.46	Joback Method
dvisc	0.0043249	Pa×s	244.46	Joback Method
dvisc	0.0011778	Pa×s	312.96	Joback Method
dvisc	0.0020836	Pa×s	278.71	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=C7425458&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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume