Ethyl 3-chlorobutanoate

Other names:	Butanoic acid, 3-chloro-, ethyl ester
	Ethyl «beta»-chlorobutyrate
Inchi:	InChI=1S/C6H11ClO2/c1-3-9-6(8)4-5(2)7/h5H,3-4H2,1-2H3
InchiKey:	ZSWGSCUZUONRDN-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CCOC(=O)CC(C)Cl
Mol. weight [g/mol]:	150.60
CAS:	7425-48-1

Physical Properties

Property code	Value	Unit	Source
chl	-3384.00	kJ/mol	NIST Webbook
gf	-248.65	kJ/mol	Joback Method
hf	-432.99	kJ/mol	Joback Method
hfus	14.76	kJ/mol	Joback Method
hvap	42.10	kJ/mol	Joback Method
log10ws	-1.46		Crippen Method
logp	1.567		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	948.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	955.00		NIST Webbook
tb	449.96	K	Joback Method
tc	638.50	K	Joback Method
tf	244.46	K	Joback Method
vc	0.439	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.04	J/mol×K	449.96	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
cpg	278.93	J/mol×K	638.50	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	0.0007450	Pa×s	347.21	Joback Method
dvisc	0.0011778	Pa×s	312.96	Joback Method
dvisc	0.0020836	Pa×s	278.71	Joback Method
dvisc	0.0043249	Pa×s	244.46	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7425481&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
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume