

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	955.00		NIST Webbook
rinpol	947.00		NIST Webbook
tb	449.96	K	Joback Method
tc	638.50	K	Joback Method
tf	244.46	K	Joback Method
vc	0.439	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.04	J/mol×K	449.96	Joback Method
cpg	234.96	J/mol×K	481.38	Joback Method

cpg	244.50	J/molxK	512.81	Joback Method
cpg	253.66	J/molxK	544.23	Joback Method
cpg	262.46	J/molxK	575.65	Joback Method
cpg	270.88	J/molxK	607.08	Joback Method
cpg	278.93	J/molxK	638.50	Joback Method
dvisc	0.0043249	Paxs	244.46	Joback Method
dvisc	0.0020836	Paxs	278.71	Joback Method
dvisc	0.0011778	Paxs	312.96	Joback Method
dvisc	0.0007450	Paxs	347.21	Joback Method
dvisc	0.0005117	Paxs	381.46	Joback Method
dvisc	0.0003739	Paxs	415.71	Joback Method
dvisc	0.0002866	Paxs	449.96	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C7425481&Units=SI

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

Latest version available from:

<https://www.chemeo.com/cid/26-482-8/Ethyl-3-chlorobutanoate.pdf>

Generated by Cheméo on 2024-04-23 09:44:05.03658723 +0000 UTC m=+16154693.957164541.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.