(+/-)-ETHYL 2-CHLOROPROPIONATE

Other names: 2-Chloropropionic acid, ethyl ester
Ethyl 2-chloropropanoate
Ethyl 2-chloropropionate
Ethyl «alpha»-chloropropionate
Propionic acid, 2-chloro-, ethyl ester
UN 2935

Inchi: InChI=1S/C5H9ClO2/c1-3-8-5(7)4(2)6/h4H,3H2,1-2H3

InchiKey: JEAVBVKAYUCPAQ-UHFFFAOYSA-N

Formula: C5H9ClO2

SMILES: CCOC(=O)C(C)Cl

Mol. weight [g/mol]: 136.58

CAS: 535-13-7

Physical Properties

Property code	Value	Unit	Source
af	0.3798		Cheméo Relay (1.0)
chl	-2737.00	kJ/mol	NIST Webbook
chl	-2761.90 ± 2.10	kJ/mol	NIST Webbook
gf	-257.07	kJ/mol	Joback Method
hf	-514.08	kJ/mol	Cheméo Relay (1.0)
hfus	12.17	kJ/mol	Joback Method
hvap	44.22	kJ/mol	Cheméo Relay (1.0)
ie	10.39	eV	Cheméo Relay (1.0)
log10ws	-1.10		Cheméo Relay (1.0)
logp	1.177		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	3538.87	kPa	Joback Method
rinpol	848.00		NIST Webbook
rinpol	851.00		NIST Webbook
rinpol	857.00		NIST Webbook
rinpol	838.00		NIST Webbook
rinpol	841.00		NIST Webbook
rinpol	832.00		NIST Webbook
rinpol	857.00		NIST Webbook
ripol	1290.00		NIST Webbook
ripol	1250.00		NIST Webbook
ripol	1229.00		NIST Webbook

ripol	1254.00		NIST Webbook
ripol	1288.00		NIST Webbook
ripol	1232.00		NIST Webbook
ripol	1226.00		NIST Webbook
tb	420.70	K	NIST Webbook
tc	589.59	K	Cheméo Relay (1.0)
tf	227.40	K	Cheméo Relay (1.0)
vc	0.376	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	186.92	J/mol×K	427.08	Joback Method
cpg	195.50	J/mol×K	458.81	Joback Method
cpg	203.77	J/mol×K	490.53	Joback Method
cpg	211.73	J/mol×K	522.26	Joback Method
cpg	219.39	J/mol×K	553.98	Joback Method
cpg	226.73	J/mol×K	585.71	Joback Method
cpg	233.77	J/mol×K	617.43	Joback Method
cpl	220.50	J/mol×K	298.00	NIST Webbook
dvisc	0.0042591	Pa×s	233.19	Joback Method
dvisc	0.0020958	Pa×s	265.50	Joback Method
dvisc	0.0012028	Pa×s	297.82	Joback Method
dvisc	0.0007696	Pa×s	330.13	Joback Method
dvisc	0.0005332	Pa×s	362.45	Joback Method
dvisc	0.0003923	Pa×s	394.76	Joback Method
dvisc	0.0003024	Pa×s	427.08	Joback Method
hvapt	46.50	kJ/mol	349.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38125e+01
Coeff. B	-4.00138e+03
Coeff. C	-1.90580e+01
Temperature range (K), min.	274.55

Temperature range (K), max.	489.75

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C535137&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
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor 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