Acetic acid, dichloro-, ethyl ester

Other names:	Dichloroacetic acid, ethyl ester
	Ethyl 2,2-dichloroacetate
	Ethyl dichloroacetate
	Ethyl dichloroethanoate
Inchi:	InChI=1S/C4H6Cl2O2/c1-2-8-4(7)3(5)6/h3H,2H2,1H3
InchiKey:	IWYBVQLPTCMVFO-UHFFFAOYSA-N
Formula:	C4H6Cl2O2
SMILES:	CCOC(=O)C(Cl)Cl
Mol. weight [g/mol]:	157.00
CAS:	535-15-9

Physical Properties

Property code	Value	Unit	Source
chl	-1976.00	kJ/mol	NIST Webbook
chl	-1980.00 ± 8.00	kJ/mol	NIST Webbook
gf	-277.42	kJ/mol	Joback Method
hf	-407.45	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	38.00	kJ/mol	NIST Webbook
hvap	50.60 ± 0.10	kJ/mol	NIST Webbook
hvap	50.60 ± 0.04	kJ/mol	NIST Webbook
hvap	46.20	kJ/mol	NIST Webbook
hvap	50.60	kJ/mol	NIST Webbook
log10ws	-1.27		Crippen Method
logp	1.353		Crippen Method
mcvol	99.140	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
rinpol	871.00		NIST Webbook
rinpol	882.40		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	871.00		NIST Webbook
rinpol	904.00		NIST Webbook
rinpol	887.00		NIST Webbook
rinpol	869.00		NIST Webbook
rinpol	872.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1423.00		NIST Webbook

ripol	1384.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1396.00		NIST Webbook
tb	441.63	K	Joback Method
tc	640.84	K	Joback Method
tf	251.84	K	Joback Method
vc	0.376	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.22	J/mol×K	640.84	Joback Method
cpg	203.72	J/mol×K	607.64	Joback Method
cpg	197.95	J/mol×K	574.44	Joback Method
cpg	191.90	J/mol×K	541.23	Joback Method
cpg	185.57	J/mol×K	508.03	Joback Method
cpg	178.98	J/mol×K	474.83	Joback Method
cpg	172.11	J/mol×K	441.63	Joback Method
cpl	209.60	J/mol×K	298.00	NIST Webbook
dvisc	0.0004356	Pa×s	410.00	Joback Method
dvisc	0.0005838	Pa×s	378.37	Joback Method
dvisc	0.0008253	Pa×s	346.74	Joback Method
dvisc	0.0012506	Pa×s	315.10	Joback Method
dvisc	0.0020794	Pa×s	283.47	Joback Method
dvisc	0.0039286	Pa×s	251.84	Joback Method
dvisc	0.0003390	Pa×s	441.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.25687e+01
Coeff. B	-3.92264e+03
Coeff. C	1.80800e+00
Temperature range (K), min.	275.75
Temperature range (K), max.	538.71

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C535159&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

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
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