Acetic acid, trichloro-, ethyl ester

Other names:	Acetic acid, 2,2,2-trichloroethyl ester
	Acetic acid, ester with trichloroethanol
	Ethyl trichloroacetate
	Trichloroethyl acetate
Inchi:	InChI=1S/C4H5Cl3O2/c1-2-9-3(8)4(5,6)7/h2H2,1H3
InchiKey:	SJMLNDPIJZBEKY-UHFFFAOYSA-N
Formula:	C4H5Cl3O2
SMILES:	CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	191.44
CAS:	515-84-4

Physical Properties

Property code	Value	Unit	Source
affp	790.40	kJ/mol	NIST Webbook
basg	759.40	kJ/mol	NIST Webbook
chl	-1872.00	kJ/mol	NIST Webbook
chl	-1879.00 ± 8.00	kJ/mol	NIST Webbook
gf	-284.07	kJ/mol	Joback Method
hf	-426.66	kJ/mol	Joback Method
hfus	14.08	kJ/mol	Joback Method
hvap	50.97 ± 0.12	kJ/mol	NIST Webbook
hvap	51.00 ± 0.10	kJ/mol	NIST Webbook
log10ws	-1.92		Crippen Method
logp	1.920		Crippen Method
mcvol	111.380	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
rinpol	930.00		NIST Webbook
rinpol	955.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	961.70		NIST Webbook
rinpol	990.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	944.00		NIST Webbook

rinpol	981.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	965.00		NIST Webbook
ripol	1400.00		NIST Webbook
ripol	1390.00		NIST Webbook
ripol	1396.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1443.00		NIST Webbook
tb	440.70	K	NIST Webbook
tc	690.53	K	Joback Method
tf	299.18	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.64	J/mol×K	476.27	Joback Method
cpg	226.33	J/mol×K	654.82	Joback Method
cpg	221.07	J/mol×K	619.11	Joback Method
cpg	215.39	J/mol×K	583.40	Joback Method
cpg	209.27	J/mol×K	547.69	Joback Method
cpg	202.69	J/mol×K	511.98	Joback Method
cpg	231.19	J/mol×K	690.53	Joback Method
cpl	230.10	J/mol×K	298.00	NIST Webbook
dvisc	0.0033897	Pa×s	299.18	Joback Method
dvisc	0.0003575	Pa×s	476.27	Joback Method
dvisc	0.0004595	Pa×s	446.75	Joback Method
dvisc	0.0006120	Pa×s	417.24	Joback Method
dvisc	0.0008515	Pa×s	387.73	Joback Method
dvisc	0.0012509	Pa×s	358.21	Joback Method
dvisc	0.0019690	Pa×s	328.69	Joback Method
hvapt	49.00	kJ/mol	366.50	NIST Webbook
hvapt	47.50	kJ/mol	342.50	NIST Webbook

Correlations

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.07732e+01
Coeff. B	-3.23263e+03
Coeff. C	-2.22620e+01
Temperature range (K), min.	288.45
Temperature range (K), max.	614.13

Sources

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=C515844&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
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