Acetic acid, trichloro-, methyl ester

Other names:	Methyl trichloroacetate
	UN 2533
Inchi:	InChI=1S/C3H3Cl3O2/c1-8-2(7)3(4,5)6/h1H3
InchiKey:	VHFUHRXYRYWELT-UHFFFAOYSA-N
Formula:	C3H3Cl3O2
SMILES:	COC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	177.41
CAS:	598-99-2

Physical Properties

Property code	Value	Unit	Source
chl	-1211.00	kJ/mol	NIST Webbook
chl	-1218.00 ± 8.00	kJ/mol	NIST Webbook
gf	-292.49	kJ/mol	Joback Method
hf	-406.02	kJ/mol	Joback Method
hfus	11.49	kJ/mol	Joback Method
hvap	48.30 ± 0.10	kJ/mol	NIST Webbook
hvap	48.33 ± 0.12	kJ/mol	NIST Webbook
log10ws	-1.50		Crippen Method
logp	1.530		Crippen Method
mcvol	97.290	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	876.00		NIST Webbook
rinpol	867.00		NIST Webbook
rinpol	884.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	895.50		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	875.00		NIST Webbook
rinpol	897.00		NIST Webbook
rinpol	896.00		NIST Webbook
rinpol	934.00		NIST Webbook
ripol	1387.00		NIST Webbook

ripol	1387.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1387.00		NIST Webbook
ripol	1378.00		NIST Webbook
tb	425.70	K	NIST Webbook
tb	427.00	K	NIST Webbook
tb	427.00 ± 3.00	K	NIST Webbook
tb	427.00 ± 0.20	K	NIST Webbook
tc	670.81	K	Joback Method
tf	255.70 ± 0.40	K	NIST Webbook
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.77	J/mol×K	453.39	Joback Method
cpg	164.37	J/mol×K	489.63	Joback Method
cpg	169.57	J/mol×K	525.86	Joback Method
cpg	174.38	J/mol×K	562.10	Joback Method
cpg	178.81	J/mol×K	598.34	Joback Method
cpg	182.89	J/mol×K	634.58	Joback Method
cpg	186.63	J/mol×K	670.81	Joback Method
dvisc	0.0035022	Pa×s	287.91	Joback Method
dvisc	0.0020802	Pa×s	315.49	Joback Method
dvisc	0.0013435	Pa×s	343.07	Joback Method
dvisc	0.0009260	Pa×s	370.65	Joback Method
dvisc	0.0006720	Pa×s	398.23	Joback Method
dvisc	0.0005084	Pa×s	425.81	Joback Method
dvisc	0.0003979	Pa×s	453.39	Joback Method

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=C598992&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume