Trichloroaetic acid isopropyl ester

Other names:	Acetic acid, trichloro-, 1-methylethyl ester
	Acetic acid, trichloro-, isopropyl ester
	Isopropyl trichloroacetate
	1-Methylethyl trichloroacetate
	Trichloroacetic acid, isopropyl ester
Inchi:	InChI=1S/C5H7Cl3O2/c1-3(2)10-4(9)5(6,7)8/h3H,1-2H3
InchiKey:	JYXIYFNAIFVCAN-UHFFFAOYSA-N
Formula:	C5H7Cl3O2
SMILES:	CC(C)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	205.47
CAS:	3974-99-0

Physical Properties

Property code	Value	Unit	Source
chl	-2492.00	kJ/mol	NIST Webbook
chl	-2500.90 ± 4.20	kJ/mol	NIST Webbook
gf	-278.09	kJ/mol	Joback Method
hf	-484.50 ± 9.60	kJ/mol	NIST Webbook
hfl	-536.40 ± 8.40	kJ/mol	NIST Webbook
hfus	13.15	kJ/mol	Joback Method
hvap	51.90 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.45		Crippen Method
logp	2.308		Crippen Method
mcvol	125.470	ml/mol	McGowan Method
pc	3318.18	kPa	Joback Method
rinpol	995.90		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1312.00		NIST Webbook
ripol	1312.00		NIST Webbook
tb	498.71	K	Joback Method
tc	714.64	K	Joback Method
tf	295.45	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.95	J/mol×K	498.71	Joback Method
cpg	243.58	J/mol×K	534.70	Joback Method
cpg	251.62	J/mol×K	570.69	Joback Method
cpg	259.12	J/mol×K	606.67	Joback Method
cpg	266.09	J/mol×K	642.66	Joback Method
cpg	272.55	J/mol×K	678.65	Joback Method
cpg	278.53	J/mol×K	714.64	Joback Method
dvisc	0.0043997	Pa×s	295.45	Joback Method
dvisc	0.0022377	Pa×s	329.33	Joback Method
dvisc	0.0012911	Pa×s	363.20	Joback Method
dvisc	0.0008182	Pa×s	397.08	Joback Method
dvisc	0.0005571	Pa×s	430.96	Joback Method
dvisc	0.0004011	Pa×s	464.83	Joback Method
dvisc	0.0003020	Pa×s	498.71	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3974990&Units=SI

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

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

hfl: Liquid phase 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