Trichloroacetic acid 2-propenyl ester

Other names:	Allyl trichloroacetate
	Acetic acid, trichloro-, allyl ester
	Acetic acid, trichloro-, 2-propenyl ester
	Trichloroacetic acid allyl ester
Inchi:	InChI=1S/C5H5Cl3O2/c1-2-3-10-4(9)5(6,7)8/h2H,1,3H2
InchiKey:	LJQCONXCOYBYIE-UHFFFAOYSA-N
Formula:	C5H5Cl3O2
SMILES:	C=CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	203.45
CAS:	6304-34-3

Physical Properties

Property code	Value	Unit	Source
chl	-2349.00	kJ/mol	NIST Webbook
chl	-2356.00 ± 4.00	kJ/mol	NIST Webbook
gf	-187.81	kJ/mol	Joback Method
hf	-343.00 ± 9.60	kJ/mol	NIST Webbook
hfl	-395.00 ± 8.40	kJ/mol	NIST Webbook
hfus	15.39	kJ/mol	Joback Method
hvap	52.30 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.086		Crippen Method
mcvol	121.170	ml/mol	McGowan Method
pc	3452.08	kPa	Joback Method
rinpol	1044.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1027.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1027.00		NIST Webbook
ripol	1467.00		NIST Webbook
ripol	1467.00		NIST Webbook
tb	495.83	K	Joback Method
tc	711.57	K	Joback Method
tf	308.69	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.41	J/mol×K	495.83	Joback Method
cpg	249.72	J/mol×K	675.61	Joback Method
cpg	244.25	J/mol×K	639.66	Joback Method
cpg	238.31	J/mol×K	603.70	Joback Method
cpg	231.88	J/mol×K	567.74	Joback Method
cpg	224.92	J/mol×K	531.79	Joback Method
cpg	254.75	J/mol×K	711.57	Joback Method
dvisc	0.0003259	Pa×s	495.83	Joback Method
dvisc	0.0004180	Pa×s	464.64	Joback Method
dvisc	0.0005558	Pa×s	433.45	Joback Method
dvisc	0.0007722	Pa×s	402.26	Joback Method
dvisc	0.0011340	Pa×s	371.07	Joback Method
dvisc	0.0017869	Pa×s	339.88	Joback Method
dvisc	0.0030869	Pa×s	308.69	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=C6304343&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
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