Trichloroacetic acid 2-methylpropyl ester

Other names:	Isobutyl trichloroacetate
	Acetic acid, trichloro-, isobutyl ester
	Acetic acid, trichloro-, 2-methylpropyl ester
	Trichloroacetic acid isobutyl ester
Inchi:	InChI=1S/C6H9Cl3O2/c1-4(2)3-11-5(10)6(7,8)9/h4H,3H2,1-2H3
InchiKey:	LRASRNYGUIRRSW-UHFFFAOYSA-N
Formula:	C6H9Cl3O2
SMILES:	CC(C)COC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]:	219.49
CAS:	33560-15-5

Physical Properties

Property code	Value	Unit	Source
chl	-3154.00	kJ/mol	NIST Webbook
chl	-3160.80 ± 8.40	kJ/mol	NIST Webbook
gf	-269.67	kJ/mol	Joback Method
hf	-500.80 ± 9.60	kJ/mol	NIST Webbook
hfl	-554.00 ± 8.40	kJ/mol	NIST Webbook
hfus	15.74	kJ/mol	Joback Method
hvap	53.10 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.52		Crippen Method
logp	2.556		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1103.80		NIST Webbook
rinpol	1106.00		NIST Webbook
rinpol	1106.00		NIST Webbook
ripol	1425.00		NIST Webbook
ripol	1425.00		NIST Webbook
tb	521.59	K	Joback Method
tc	734.09	K	Joback Method
tf	306.72	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	276.03	J/mol×K	521.59	Joback Method
cpg	318.90	J/mol×K	698.67	Joback Method
cpg	311.49	J/mol×K	663.25	Joback Method
cpg	303.52	J/mol×K	627.84	Joback Method
cpg	294.97	J/mol×K	592.42	Joback Method
cpg	285.82	J/mol×K	557.01	Joback Method
cpg	325.79	J/mol×K	734.09	Joback Method
dvisc	0.0002670	Pa×s	521.59	Joback Method
dvisc	0.0003560	Pa×s	485.78	Joback Method
dvisc	0.0004970	Pa×s	449.97	Joback Method
dvisc	0.0007350	Pa×s	414.16	Joback Method
dvisc	0.0011705	Pa×s	378.34	Joback Method
dvisc	0.0020546	Pa×s	342.53	Joback Method
dvisc	0.0041126	Pa×s	306.72	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33560155&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