Trichloroacetic acid 3-methylbutyl ester

Other names: Acetic acid, trichloro-, 3-methylbutyl ester
3-Methylbutyl trichloroacetate
Isopentyl trichloroacetate
Inchi: InChI=1S/C7H11Cl3O2/c1-5(2)3-4-12-6(11)7(8,9)10/h5H,3-4H2,1-2H3
InchiKey: HBNLTLLITHPMDZ-UHFFFAOYSA-N
Formula: C7H11Cl3O2
SMILES: CC(C)CCOC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 233.52
CAS: 57392-55-9

Physical Properties

Property code	Value	Unit	Source
chl	-3811.70 ± 4.20	kJ/mol	NIST Webbook
chl	-3805.00	kJ/mol	NIST Webbook
gf	-261.25	kJ/mol	Joback Method
hf	-523.40 ± 9.60	kJ/mol	NIST Webbook
hfl	-581.20 ± 8.40	kJ/mol	NIST Webbook
hfus	18.33	kJ/mol	Joback Method
hvap	57.70 ± 4.20	kJ/mol	NIST Webbook
log10ws	-2.93		Crippen Method
logp	2.946		Crippen Method
mcvol	153.650	ml/mol	McGowan Method
pc	2690.21	kPa	Joback Method
rinpol	1208.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1203.30		NIST Webbook
rinpol	1208.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1532.00		NIST Webbook
tb	544.47	K	Joback Method
tc	753.60	K	Joback Method
tf	317.99	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.04	J/mol×K	544.47	Joback Method
cpg	366.56	J/mol×K	718.74	Joback Method
cpg	358.30	J/mol×K	683.89	Joback Method
cpg	349.44	J/mol×K	649.03	Joback Method
cpg	339.96	J/mol×K	614.18	Joback Method
cpg	329.84	J/mol×K	579.32	Joback Method
cpg	374.25	J/mol×K	753.60	Joback Method
dvisc	0.0002349	Pa×s	544.47	Joback Method
dvisc	0.0003144	Pa×s	506.72	Joback Method
dvisc	0.0004410	Pa×s	468.98	Joback Method
dvisc	0.0006562	Pa×s	431.23	Joback Method
dvisc	0.0010540	Pa×s	393.48	Joback Method
dvisc	0.0018721	Pa×s	355.74	Joback Method
dvisc	0.0038109	Pa×s	317.99	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57392559&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