Isobutyric acid, 2,2,2-trichloroethyl ester

Other names: 2,2,2-Trichloroethyl isobutanoate
Propanoic acid, 2-methyl, 2,2,2-trichloroethyl ester
2,2,2-Trichloroethyl 2-methylpropanoate
Inchi: InChI=1S/C6H9Cl3O2/c1-4(2)5(10)11-3-6(7,8)9/h4H,3H2,1-2H3
InchiKey: QNYXMOBLXOMWCE-UHFFFAOYSA-N
Formula: C6H9Cl3O2
SMILES: CC(C)C(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 219.49

Physical Properties

Property code	Value	Unit	Source
gf	-269.67	kJ/mol	Joback Method
hf	-473.22	kJ/mol	Joback Method
hfus	15.74	kJ/mol	Joback Method
hvap	49.58	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.556		Crippen Method
mcvol	139.560	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
rinpol	1102.00		NIST Webbook
rinpol	1153.00		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	285.82	J/mol×K	557.01	Joback Method
cpg	294.97	J/mol×K	592.42	Joback Method
cpg	303.52	J/mol×K	627.84	Joback Method
cpg	311.49	J/mol×K	663.25	Joback Method

cpg	318.90	J/mol×K	698.67	Joback Method
cpg	325.79	J/mol×K	734.09	Joback Method
dvisc	0.0041126	Pa×s	306.72	Joback Method
dvisc	0.0020546	Pa×s	342.53	Joback Method
dvisc	0.0011705	Pa×s	378.34	Joback Method
dvisc	0.0007350	Pa×s	414.16	Joback Method
dvisc	0.0004970	Pa×s	449.97	Joback Method
dvisc	0.0003560	Pa×s	485.78	Joback Method
dvisc	0.0002670	Pa×s	521.59	Joback Method

Sources

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=U354634&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume