Propanoic acid, 2,2-dichloro-, butyl ester

Other names:	Propionic acid, 2,2-dichloro-, butyl ester
	Butyl «alpha»,«alpha»-dichloropropionate
Inchi:	InChI=1S/C7H12Cl2O2/c1-3-4-5-11-6(10)7(2,8)9/h3-5H2,1-2H3
InchiKey:	INWCHAUMYGSQAZ-UHFFFAOYSA-N
Formula:	C7H12Cl2O2
SMILES:	CCCCOC(=O)C(C)(Cl)Cl
Mol. weight [g/mol]:	199.07
CAS:	17640-07-2

Physical Properties

Property code	Value	Unit	Source
gf	-246.88	kJ/mol	Joback Method
hf	-472.84	kJ/mol	Joback Method
hfus	17.65	kJ/mol	Joback Method
hvap	47.81	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.524		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2773.00	kPa	Joback Method
tb	507.48	K	Joback Method
tc	707.27	K	Joback Method
tf	303.07	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.12	J/mol×K	507.48	Joback Method
cpg	305.33	J/mol×K	540.78	Joback Method
cpg	315.93	J/mol×K	574.08	Joback Method
cpg	325.92	J/mol×K	607.38	Joback Method
cpg	335.33	J/mol×K	640.67	Joback Method
cpg	344.19	J/mol×K	673.97	Joback Method
cpg	352.51	J/mol×K	707.27	Joback Method

dvisc	0.0034763	Pa×s	303.07	Joback Method
dvisc	0.0018321	Pa×s	337.14	Joback Method
dvisc	0.0010860	Pa×s	371.21	Joback Method
dvisc	0.0007029	Pa×s	405.28	Joback Method
dvisc	0.0004867	Pa×s	439.34	Joback Method
dvisc	0.0003553	Pa×s	473.41	Joback Method
dvisc	0.0002706	Pa×s	507.48	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=C17640072&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume