Isopropyl, a,a-dichloropropionate

Other names:	Isopropyl «alpha»,«alpha»-dichloropropionate
	Isopropyl, alpha,alpha-dichloropropionate
	Isopropyl, a,a-dichloropropionate
Inchi:	InChI=1S/C6H10Cl2O2/c1-4(2)10-5(9)6(3,7)8/h4H,1-3H3
InchiKey:	QVZCJUSIWAGBDX-UHFFFAOYSA-N
Formula:	C6H10Cl2O2
SMILES:	CC(C)OC(=O)C(C)(Cl)Cl
Mol. weight [g/mol]:	185.05

Physical Properties

Property code	Value	Unit	Source
hf	-538.65	kJ/mol	Cheméo Relay (1.0)
hfus	11.54	kJ/mol	Joback Method
hvap	48.42	kJ/mol	Cheméo Relay (1.0)
ie	10.36	eV	Cheméo Relay (1.0)
log10ws	-2.45		Cheméo Relay (1.0)
logp	2.132		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	422.42	K	Cheméo Relay (1.0)
tc	621.95	K	Cheméo Relay (1.0)
tf	252.39	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.57	J/mol×K	484.16	Joback Method
cpg	263.03	J/mol×K	518.69	Joback Method
cpg	272.88	J/mol×K	553.22	Joback Method
cpg	282.14	J/mol×K	587.75	Joback Method
cpg	290.84	J/mol×K	622.28	Joback Method
cpg	298.99	J/mol×K	656.81	Joback Method
cpg	306.61	J/mol×K	691.34	Joback Method
dvisc	0.0051343	Pa×s	276.80	Joback Method

dvisc	0.0024308	Pa×s	311.36	Joback Method
dvisc	0.0013363	Pa×s	345.92	Joback Method
dvisc	0.0008189	Pa×s	380.48	Joback Method
dvisc	0.0005445	Pa×s	415.04	Joback Method
dvisc	0.0003855	Pa×s	449.60	Joback Method
dvisc	0.0002867	Pa×s	484.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54587483&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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