

Propanoic acid, 2,2-dichloro-, 1-methylethyl ester

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
CAS:	54587-48-3

Physical Properties

Property code	Value	Unit	Source
gf	-257.74	kJ/mol	Joback Method
hf	-457.48	kJ/mol	Joback Method
hfus	11.54	kJ/mol	Joback Method
hvap	45.19	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.132		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
tb	484.16	K	Joback Method
tc	691.34	K	Joback Method
tf	276.80	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.57	J/molxK	484.16	Joback Method
cpg	263.03	J/molxK	518.69	Joback Method
cpg	272.88	J/molxK	553.22	Joback Method
cpg	282.14	J/molxK	587.75	Joback Method
cpg	290.84	J/molxK	622.28	Joback Method
cpg	298.99	J/molxK	656.81	Joback Method

cpg	306.61	J/mol×K	691.34	Joback Method
dvisc	0.0051343	Paxs	276.80	Joback Method
dvisc	0.0024308	Paxs	311.36	Joback Method
dvisc	0.0013363	Paxs	345.92	Joback Method
dvisc	0.0008189	Paxs	380.48	Joback Method
dvisc	0.0005445	Paxs	415.04	Joback Method
dvisc	0.0003855	Paxs	449.60	Joback Method
dvisc	0.0002867	Paxs	484.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54587483&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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