Propanoic acid, 2,3-dichloro-, 1-methylethyl ester

Other names: Isopropyl 2,3-dichloropropionate
Propionic acid, 2,3-dichloro-, isopropyl ester
Isopropyl-alpha,beta-dichloro propionate
Isopropyl 2,3-dichloropropanoate

Inchi: InChI=1S/C6H10Cl2O2/c1-4(2)10-6(9)5(8)3-7/h4-5H,3H2,1-2H3

InchiKey: DQNKZNXCBULFCV-UHFFFAOYSA-N

Formula: C6H10Cl2O2

SMILES: CC(C)OC(=O)C(Cl)CCl

Mol. weight [g/mol]: 185.05

CAS: 54774-99-1

Physical Properties

Property code	Value	Unit	Source
gf	-263.02	kJ/mol	Joback Method
hf	-454.01	kJ/mol	Joback Method
hfus	15.43	kJ/mol	Joback Method
hvap	46.10	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.784		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1032.00		NIST Webbook
rinpol	1032.00		NIST Webbook
ripol	1494.00		NIST Webbook
ripol	1494.00		NIST Webbook
tb	486.95	K	Joback Method
tc	685.84	K	Joback Method
tf	259.38	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.45	J/mol×K	486.95	Joback Method

cpg	294.25	J/mol×K	652.69	Joback Method
cpg	286.16	J/mol×K	619.54	Joback Method
cpg	277.63	J/mol×K	586.39	Joback Method
cpg	268.68	J/mol×K	553.25	Joback Method
cpg	259.28	J/mol×K	520.10	Joback Method
cpg	301.92	J/mol×K	685.84	Joback Method
dvisc	0.0002759	Pa×s	486.95	Joback Method
dvisc	0.0003681	Pa×s	449.02	Joback Method
dvisc	0.0005180	Pa×s	411.09	Joback Method
dvisc	0.0007812	Pa×s	373.16	Joback Method
dvisc	0.0012930	Pa×s	335.24	Joback Method
dvisc	0.0024337	Pa×s	297.31	Joback Method
dvisc	0.0055114	Pa×s	259.38	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=C54774991&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume