Propanoic acid, 2-chloro-, 1,1-dimethylethyl ester

Inchi: InChI=1S/C7H13ClO2/c1-5(8)6(9)10-7(2,3)4/h5H,1-4H3
InchiKey: YXYWJZNXZGYLNO-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CC(Cl)C(=O)OC(C)(C)C
Mol. weight [g/mol]: 164.63

Physical Properties

Property code	Value	Unit	Source
gf	-237.39	kJ/mol	Joback Method
hf	-462.38	kJ/mol	Joback Method
hfus	9.93	kJ/mol	Joback Method
hvap	43.03	kJ/mol	Joback Method
log10ws	-1.99		Crippen Method
logp	1.955		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	905.00		NIST Webbook
rinpol	911.00		NIST Webbook
rinpol	917.00		NIST Webbook
rinpol	921.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	911.00		NIST Webbook
ripol	1223.00		NIST Webbook
ripol	1229.00		NIST Webbook
ripol	1264.00		NIST Webbook
ripol	1229.00		NIST Webbook
ripol	1220.00		NIST Webbook
tb	469.61	K	Joback Method
tc	668.23	K	Joback Method
tf	258.15	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.41	J/mol×K	469.61	Joback Method
cpg	280.59	J/mol×K	502.71	Joback Method
cpg	292.14	J/mol×K	535.82	Joback Method
cpg	303.08	J/mol×K	568.92	Joback Method
cpg	313.42	J/mol×K	602.02	Joback Method
cpg	323.19	J/mol×K	635.13	Joback Method
cpg	332.40	J/mol×K	668.23	Joback Method
dvisc	0.0060606	Pa×s	258.15	Joback Method
dvisc	0.0026380	Pa×s	293.39	Joback Method
dvisc	0.0013725	Pa×s	328.64	Joback Method
dvisc	0.0008105	Pa×s	363.88	Joback Method
dvisc	0.0005252	Pa×s	399.12	Joback Method
dvisc	0.0003652	Pa×s	434.37	Joback Method
dvisc	0.0002682	Pa×s	469.61	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=U132238&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