Propanoic acid, 3-chloro, 1,1-dimethylethyl ester

Inchi: InChI=1S/C7H13ClO2/c1-7(2,3)10-6(9)4-5-8/h4-5H2,1-3H3
InchiKey: PGULCJLBEJUCRO-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CC(C)(C)OC(=O)CCCl
Mol. weight [g/mol]: 164.63

Physical Properties

Property code	Value	Unit	Source
gf	-234.95	kJ/mol	Joback Method
hf	-457.10	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	43.42	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.957		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	991.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	973.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1368.00		NIST Webbook
tb	470.05	K	Joback Method
tc	664.25	K	Joback Method
tf	273.15	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	268.23	J/mol×K	470.05	Joback Method
cpg	280.06	J/mol×K	502.42	Joback Method
cpg	291.30	J/mol×K	534.78	Joback Method
cpg	301.96	J/mol×K	567.15	Joback Method
cpg	312.05	J/mol×K	599.52	Joback Method
cpg	321.60	J/mol×K	631.88	Joback Method
cpg	330.63	J/mol×K	664.25	Joback Method
dvisc	0.0041252	Pa×s	273.15	Joback Method
dvisc	0.0020752	Pa×s	305.97	Joback Method
dvisc	0.0011926	Pa×s	338.78	Joback Method
dvisc	0.0007558	Pa×s	371.60	Joback Method
dvisc	0.0005158	Pa×s	404.42	Joback Method
dvisc	0.0003728	Pa×s	437.23	Joback Method
dvisc	0.0002819	Pa×s	470.05	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R113687&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
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