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

Inchi: InChI=1S/C8H15ClO2/c1-5(2)7(4)11-8(10)6(3)9/h5-7H,1-4H3
InchiKey: CERNFPCEYCDJQG-UHFFFAOYSA-N
Formula: C8H15ClO2
SMILES: CC(Cl)C(=O)OC(C)C(C)C
Mol. weight [g/mol]: 178.66

Physical Properties

Property code	Value	Unit	Source
gf	-236.69	kJ/mol	Joback Method
hf	-484.83	kJ/mol	Joback Method
hfus	12.89	kJ/mol	Joback Method
hvap	45.78	kJ/mol	Joback Method
log10ws	-2.17		Crippen Method
logp	2.201		Crippen Method
mcvol	143.260	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
rinpol	1046.00		NIST Webbook
rinpol	1044.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1054.00		NIST Webbook
ripol	1369.00		NIST Webbook
ripol	1366.00		NIST Webbook
ripol	1386.00		NIST Webbook
ripol	1368.00		NIST Webbook
tb	494.84	K	Joback Method
tc	687.55	K	Joback Method
tf	237.00	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.34	J/mol×K	494.84	Joback Method

cpg	321.20	J/mol×K	526.96	Joback Method
cpg	333.50	J/mol×K	559.08	Joback Method
cpg	345.26	J/mol×K	591.20	Joback Method
cpg	356.48	J/mol×K	623.32	Joback Method
cpg	367.16	J/mol×K	655.43	Joback Method
cpg	377.31	J/mol×K	687.55	Joback Method
dvisc	0.0096797	Pa×s	237.00	Joback Method
dvisc	0.0031841	Pa×s	279.97	Joback Method
dvisc	0.0014081	Pa×s	322.95	Joback Method
dvisc	0.0007542	Pa×s	365.92	Joback Method
dvisc	0.0004606	Pa×s	408.89	Joback Method
dvisc	0.0003090	Pa×s	451.87	Joback Method
dvisc	0.0002222	Pa×s	494.84	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R113667&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