Propanoic acid, 2-chloro, 1-methyl-3-butenyl ester

Inchi: InChI=1S/C8H13ClO2/c1-4-5-6(2)11-8(10)7(3)9/h4,6-7H,1,5H2,2-3H3
InchiKey: QVYJRALGDILKPA-UHFFFAOYSA-N
Formula: C8H13ClO2
SMILES: C=CCC(C)OC(=O)C(C)Cl
Mol. weight [g/mol]: 176.64

Physical Properties

Property code	Value	Unit	Source
gf	-146.41	kJ/mol	Joback Method
hf	-354.12	kJ/mol	Joback Method
hfus	15.13	kJ/mol	Joback Method
hvap	45.50	kJ/mol	Joback Method
log10ws	-2.26		Crippen Method
logp	2.121		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	1057.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1062.00		NIST Webbook
ripol	1436.00		NIST Webbook
ripol	1434.00		NIST Webbook
ripol	1438.00		NIST Webbook
ripol	1436.00		NIST Webbook
tb	491.96	K	Joback Method
tc	684.44	K	Joback Method
tf	250.24	K	Joback Method
vc	0.525	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.45	J/mol×K	491.96	Joback Method

cpg	344.52	J/mol×K	652.36	Joback Method
cpg	334.74	J/mol×K	620.28	Joback Method
cpg	324.45	J/mol×K	588.20	Joback Method
cpg	313.65	J/mol×K	556.12	Joback Method
cpg	302.32	J/mol×K	524.04	Joback Method
cpg	353.80	J/mol×K	684.44	Joback Method
dvisc	0.0002384	Pa×s	491.96	Joback Method
dvisc	0.0003194	Pa×s	451.67	Joback Method
dvisc	0.0004533	Pa×s	411.39	Joback Method
dvisc	0.0006939	Pa×s	371.10	Joback Method
dvisc	0.0011784	Pa×s	330.81	Joback Method
dvisc	0.0023178	Pa×s	290.53	Joback Method
dvisc	0.0056683	Pa×s	250.24	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R113756&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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