Propanoic acid, 2-chloro, 3-butenyl ester

Inchi: InChI=1S/C7H11ClO2/c1-3-4-5-10-7(9)6(2)8/h3,6H,1,4-5H2,2H3
InchiKey: VZLFFQDRAJPQON-UHFFFAOYSA-N
Formula: C7H11ClO2
SMILES: C=CCCOC(=O)C(C)Cl
Mol. weight [g/mol]: 162.61

Physical Properties

Property code	Value	Unit	Source
gf	-152.39	kJ/mol	Joback Method
hf	-328.20	kJ/mol	Joback Method
hfus	16.07	kJ/mol	Joback Method
hvap	43.66	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.733		Crippen Method
mcvol	124.870	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
rinpol	1024.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	998.00		NIST Webbook
ripol	1453.00		NIST Webbook
ripol	1454.00		NIST Webbook
ripol	1458.00		NIST Webbook
tb	469.52	K	Joback Method
tc	660.02	K	Joback Method
tf	253.97	K	Joback Method
vc	0.475	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.56	J/mol×K	469.52	Joback Method
cpg	296.31	J/mol×K	628.27	Joback Method

cpg	287.63	J/mol×K	596.52	Joback Method
cpg	278.52	J/mol×K	564.77	Joback Method
cpg	268.98	J/mol×K	533.02	Joback Method
cpg	258.99	J/mol×K	501.27	Joback Method
cpg	304.57	J/mol×K	660.02	Joback Method
dvisc	0.0002704	Pa×s	469.52	Joback Method
dvisc	0.0003512	Pa×s	433.60	Joback Method
dvisc	0.0004783	Pa×s	397.67	Joback Method
dvisc	0.0006924	Pa×s	361.75	Joback Method
dvisc	0.0010878	Pa×s	325.82	Joback Method
dvisc	0.0019112	Pa×s	289.89	Joback Method
dvisc	0.0039384	Pa×s	253.97	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R113776&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

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