Propanoic acid, 2-chloro, (E)-3-hexenyl ester

Inchi: InChI=1S/C9H15ClO2/c1-3-4-5-6-7-12-9(11)8(2)10/h4-5,8H,3,6-7H2,1-2H3/b5-4+
InchiKey: YLEQBTKAXAMNEF-SNAWJCMRSA-N
Formula: C9H15ClO2
SMILES: CCC=CCCOC(=O)C(C)Cl
Mol. weight [g/mol]: 190.67

Physical Properties

Property code	Value	Unit	Source
gf	-143.17	kJ/mol	Joback Method
hf	-377.69	kJ/mol	Joback Method
hfus	22.73	kJ/mol	Joback Method
hvap	48.74	kJ/mol	Joback Method
log10ws	-2.57		Crippen Method
logp	2.513		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1209.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1204.00		NIST Webbook
ripol	1627.00		NIST Webbook
ripol	1627.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1623.00		NIST Webbook
tb	522.76	K	Joback Method
tc	713.52	K	Joback Method
tf	273.19	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.35	J/mol×K	522.76	Joback Method
cpg	347.04	J/mol×K	554.55	Joback Method

cpg	359.13	J/mol×K	586.35	Joback Method
cpg	370.63	J/mol×K	618.14	Joback Method
cpg	381.57	J/mol×K	649.93	Joback Method
cpg	391.96	J/mol×K	681.73	Joback Method
cpg	401.81	J/mol×K	713.52	Joback Method
dvisc	0.0038164	Pa×s	273.19	Joback Method
dvisc	0.0016677	Pa×s	314.78	Joback Method
dvisc	0.0008841	Pa×s	356.38	Joback Method
dvisc	0.0005352	Pa×s	397.98	Joback Method
dvisc	0.0003563	Pa×s	439.57	Joback Method
dvisc	0.0002545	Pa×s	481.16	Joback Method
dvisc	0.0001917	Pa×s	522.76	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R113796&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