Propanoic acid, 3-chloro, (Z)-3-hexenyl ester

Inchi: InChI=1S/C9H15ClO2/c1-2-3-4-5-8-12-9(11)6-7-10/h3-4H,2,5-8H2,1H3/b4-3-
InchiKey: RCTBGSWMRQJSLJ-ARJAWSKDSA-N
Formula: C9H15ClO2
SMILES: CCC=CCCOC(=O)CCCl
Mol. weight [g/mol]: 190.67

Physical Properties

Property code	Value	Unit	Source
gf	-140.73	kJ/mol	Joback Method
hf	-372.41	kJ/mol	Joback Method
hfus	26.25	kJ/mol	Joback Method
hvap	49.13	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.515		Crippen Method
mcvol	153.050	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1289.00		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1295.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1279.00		NIST Webbook
rinpol	1279.00		NIST Webbook
ripol	1790.00		NIST Webbook
ripol	1780.00		NIST Webbook
ripol	1779.00		NIST Webbook
tb	523.20	K	Joback Method
tc	710.07	K	Joback Method
tf	288.19	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	334.06	J/mol×K	523.20	Joback Method

cpg	346.42	J/mol×K	554.34	Joback Method
cpg	358.22	J/mol×K	585.49	Joback Method
cpg	369.46	J/mol×K	616.63	Joback Method
cpg	380.17	J/mol×K	647.78	Joback Method
cpg	390.36	J/mol×K	678.92	Joback Method
cpg	400.04	J/mol×K	710.07	Joback Method
dvisc	0.0027621	Pa×s	288.19	Joback Method
dvisc	0.0013787	Pa×s	327.36	Joback Method
dvisc	0.0007983	Pa×s	366.53	Joback Method
dvisc	0.0005137	Pa×s	405.70	Joback Method
dvisc	0.0003572	Pa×s	444.86	Joback Method
dvisc	0.0002635	Pa×s	484.03	Joback Method
dvisc	0.0002034	Pa×s	523.20	Joback Method

Sources

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=R296316&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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