5-Chlorovaleric acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C13H23ClO2/c1-3-4-5-6-9-12(2)16-13(15)10-7-8-11-14/h6,9,12H,3-5,7-8,10-11
InchiKey: WLTIAUVTCDQKPT-RMKNXTFCSA-N
Formula: C13H23ClO2
SMILES: CCCCC=CC(C)OC(=O)CCCCCl
Mol. weight [g/mol]: 246.77

Physical Properties

Property code	Value	Unit	Source
gf	-109.49	kJ/mol	Joback Method
hf	-460.25	kJ/mol	Joback Method
hfus	33.09	kJ/mol	Joback Method
hvap	57.64	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	4.074		Crippen Method
mcvol	209.410	ml/mol	McGowan Method
pc	1740.46	kPa	Joback Method
rinpol	1654.70		NIST Webbook
rinpol	1654.70		NIST Webbook
tb	614.28	K	Joback Method
tc	796.94	K	Joback Method
tf	318.27	K	Joback Method
vc	0.810	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.98	J/mol×K	614.28	Joback Method
cpg	543.48	J/mol×K	644.72	Joback Method
cpg	558.24	J/mol×K	675.17	Joback Method
cpg	572.29	J/mol×K	705.61	Joback Method
cpg	585.64	J/mol×K	736.05	Joback Method
cpg	598.32	J/mol×K	766.50	Joback Method
cpg	610.36	J/mol×K	796.94	Joback Method
dvisc	0.0029960	Pa×s	318.27	Joback Method

dvisc	0.0012420	Pa×s	367.60	Joback Method
dvisc	0.0006342	Pa×s	416.94	Joback Method
dvisc	0.0003733	Pa×s	466.27	Joback Method
dvisc	0.0002432	Pa×s	515.61	Joback Method
dvisc	0.0001708	Pa×s	564.94	Joback Method
dvisc	0.0001269	Pa×s	614.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292477&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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