5-Chlorovaleric acid, undec-2-enyl ester

Inchi: InChI=1S/C16H29ClO2/c1-2-3-4-5-6-7-8-9-12-15-19-16(18)13-10-11-14-17/h9,12H,2-8,1
InchiKey: MMBYQPWSFIURFR-FMIVXFBMSA-N
Formula: C16H29ClO2
SMILES: CCCCCCCCC=CCOC(=O)CCCCCl
Mol. weight [g/mol]: 288.85

Physical Properties

Property code	Value	Unit	Source
gf	-81.79	kJ/mol	Joback Method
hf	-516.89	kJ/mol	Joback Method
hfus	44.38	kJ/mol	Joback Method
hvap	64.71	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	5.245		Crippen Method
mcvol	251.680	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	2053.60		NIST Webbook
rinpol	2053.60		NIST Webbook
tb	683.36	K	Joback Method
tc	860.49	K	Joback Method
tf	367.08	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.59	J/mol×K	683.36	Joback Method
cpg	705.25	J/mol×K	712.88	Joback Method
cpg	721.11	J/mol×K	742.40	Joback Method
cpg	736.21	J/mol×K	771.92	Joback Method
cpg	750.57	J/mol×K	801.44	Joback Method
cpg	764.22	J/mol×K	830.96	Joback Method
cpg	777.18	J/mol×K	860.49	Joback Method
dvisc	0.0017965	Pa×s	367.08	Joback Method

dvisc	0.0008088	Pa×s	419.79	Joback Method
dvisc	0.0004351	Pa×s	472.51	Joback Method
dvisc	0.0002651	Pa×s	525.22	Joback Method
dvisc	0.0001768	Pa×s	577.93	Joback Method
dvisc	0.0001262	Pa×s	630.65	Joback Method
dvisc	0.0000948	Pa×s	683.36	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=U292481&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume