5-Chlorovaleric acid, dodec-9-ynyl ester

Inchi: InChI=1S/C17H29ClO2/c1-2-3-4-5-6-7-8-9-10-13-16-20-17(19)14-11-12-15-18/h2,5-16H
InchiKey: RUPFATUHMIZGOQ-UHFFFAOYSA-N
Formula: C17H29ClO2
SMILES: CCC#CCCCCCCCCOC(=O)CCCCCl
Mol. weight [g/mol]: 300.86

Physical Properties

Property code	Value	Unit	Source
gf	49.21	kJ/mol	Joback Method
hf	-382.45	kJ/mol	Joback Method
hfus	49.89	kJ/mol	Joback Method
hvap	69.13	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	5.083		Crippen Method
mcvol	261.470	ml/mol	McGowan Method
pc	1391.25	kPa	Joback Method
rinpol	2205.70		NIST Webbook
rinpol	2205.70		NIST Webbook
tb	711.08	K	Joback Method
tc	896.39	K	Joback Method
tf	489.53	K	Joback Method
vc	1.022	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.03	J/mol×K	711.08	Joback Method
cpg	740.04	J/mol×K	741.96	Joback Method
cpg	756.20	J/mol×K	772.85	Joback Method
cpg	771.53	J/mol×K	803.73	Joback Method
cpg	786.07	J/mol×K	834.62	Joback Method
cpg	799.81	J/mol×K	865.50	Joback Method
cpg	812.80	J/mol×K	896.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292247&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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