5-Chlorovaleric acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C9H13ClO2/c1-3-8(2)12-9(11)6-4-5-7-10/h1,8H,4-7H2,2H3
InchiKey: DKDCXIDSBYMDQQ-UHFFFAOYSA-N
Formula: C9H13ClO2
SMILES: C#CC(C)OC(=O)CCCCCl
Mol. weight [g/mol]: 188.65

Physical Properties

Property code	Value	Unit	Source
gf	-0.32	kJ/mol	Joback Method
hf	-203.01	kJ/mol	Joback Method
hfus	25.50	kJ/mol	Joback Method
hvap	48.64	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	1.960		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	1291.10		NIST Webbook
tb	508.72	K	Joback Method
tc	703.70	K	Joback Method
tf	325.24	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.47	J/mol×K	508.72	Joback Method
cpg	329.23	J/mol×K	541.22	Joback Method
cpg	340.44	J/mol×K	573.71	Joback Method
cpg	351.11	J/mol×K	606.21	Joback Method
cpg	361.26	J/mol×K	638.70	Joback Method
cpg	370.89	J/mol×K	671.20	Joback Method
cpg	380.02	J/mol×K	703.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292473&Units=SI

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