5-Chlorovaleric acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C10H13ClO2/c1-2-3-6-9-13-10(12)7-4-5-8-11/h1,3,6H,4-5,7-9H2/b6-3+
InchiKey: ZDYVJHVEGPSABA-ZZXKWVIFSA-N
Formula: C10H13ClO2
SMILES: C#CC=CCOC(=O)CCCCCl
Mol. weight [g/mol]: 200.66

Physical Properties

Property code	Value	Unit	Source
gf	90.76	kJ/mol	Joback Method
hf	-101.15	kJ/mol	Joback Method
hfus	31.82	kJ/mol	Joback Method
hvap	51.21	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.128		Crippen Method
mcvol	158.540	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpol	1505.30		NIST Webbook
rinpol	1505.30		NIST Webbook
tb	536.20	K	Joback Method
tc	733.09	K	Joback Method
tf	346.43	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	342.94	J/mol×K	536.20	Joback Method
cpg	354.82	J/mol×K	569.01	Joback Method
cpg	366.08	J/mol×K	601.83	Joback Method
cpg	376.75	J/mol×K	634.64	Joback Method
cpg	386.84	J/mol×K	667.46	Joback Method
cpg	396.40	J/mol×K	700.27	Joback Method
cpg	405.43	J/mol×K	733.09	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=U292475&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