5-Chlorovaleric acid, 2,7-dimethylocty-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C15H23ClO2/c1-12(2)8-9-14(11-13(3)4)18-15(17)7-5-6-10-16/h13-14H,1,5-7,1

InchiKey: MABVZJMLUHQMDS-UHFFFAOYSA-N

Formula: C15H23ClO2

SMILES: C=C(C)C#CC(CC(C)C)OC(=O)CCCCCl

Mol. weight [g/mol]: 270.80

Physical Properties

Property code	Value	Unit	Source
gf	106.78	kJ/mol	Joback Method
hf	-236.09	kJ/mol	Joback Method
hfus	35.08	kJ/mol	Joback Method
hvap	63.31	kJ/mol	Joback Method
log10ws	-4.64		Crippen Method
logp	3.933		Crippen Method
mcvol	228.990	ml/mol	McGowan Method
pc	1699.10	kPa	Joback Method
rinpol	1750.80		NIST Webbook
tb	661.00	K	Joback Method
tc	860.52	K	Joback Method
tf	421.27	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.44	J/mol×K	661.00	Joback Method
cpg	606.87	J/mol×K	694.25	Joback Method
cpg	622.42	J/mol×K	727.51	Joback Method
cpg	637.13	J/mol×K	760.76	Joback Method
cpg	651.01	J/mol×K	794.01	Joback Method
cpg	664.10	J/mol×K	827.27	Joback Method
cpg	676.41	J/mol×K	860.52	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=U292479&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
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