5-Chlorovaleric acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C14H23ClO2/c1-4-5-8-13(11-12(2)3)17-14(16)9-6-7-10-15/h12-13H,4,6-7,9-11

InchiKey: LGSSOHRMKNDPBM-UHFFFAOYSA-N

Formula: C14H23ClO2

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

Mol. weight [g/mol]: 258.78

Physical Properties

Property code	Value	Unit	Source
gf	19.07	kJ/mol	Joback Method
hf	-331.09	kJ/mol	Joback Method
hfus	35.08	kJ/mol	Joback Method
hvap	61.67	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.767		Crippen Method
mcvol	219.200	ml/mol	McGowan Method
pc	1769.87	kPa	Joback Method
rinpol	1703.30		NIST Webbook
rinpol	1703.30		NIST Webbook
tb	641.56	K	Joback Method
tc	837.20	K	Joback Method
tf	425.72	K	Joback Method
vc	0.843	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	560.51	J/mol×K	641.56	Joback Method
cpg	576.80	J/mol×K	674.17	Joback Method
cpg	592.26	J/mol×K	706.77	Joback Method
cpg	606.93	J/mol×K	739.38	Joback Method
cpg	620.81	J/mol×K	771.99	Joback Method
cpg	633.92	J/mol×K	804.59	Joback Method
cpg	646.28	J/mol×K	837.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292478&Units=SI
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

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