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
hfus	35.08	kJ/mol	Joback Method
logp	3.933		Crippen Method
mcvol	228.990	ml/mol	McGowan Method
rinpol	1750.80		NIST Webbook

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292479&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices