3-Cloropropionic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Inchi: InChI=1S/C13H19ClO2/c1-10(2)5-6-12(9-11(3)4)16-13(15)7-8-14/h11-12H,1,7-9H2,2-4H

InchiKey: NJMIWJNQZFQLFM-UHFFFAOYSA-N

Formula: C13H19ClO2

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

Mol. weight [g/mol]: 242.74

Physical Properties

Property code	Value	Unit	Source
gf	89.94	kJ/mol	Joback Method
hf	-194.81	kJ/mol	Joback Method
hfus	29.90	kJ/mol	Joback Method
hvap	58.86	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.153		Crippen Method
mcvol	200.810	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	1515.00		NIST Webbook
rinpol	1515.00		NIST Webbook
tb	615.24	K	Joback Method
tc	820.28	K	Joback Method
tf	398.73	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	486.93	J/mol×K	615.24	Joback Method
cpg	502.30	J/mol×K	649.41	Joback Method
cpg	516.87	J/mol×K	683.59	Joback Method
cpg	530.65	J/mol×K	717.76	Joback Method
cpg	543.66	J/mol×K	751.93	Joback Method
cpg	555.92	J/mol×K	786.11	Joback Method
cpg	567.45	J/mol×K	820.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299217&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