3-Chloropropionic acid, 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C12H19ClO2/c1-4-5-6-11(9-10(2)3)15-12(14)7-8-13/h10-11H,4,7-9H2,1-3H3
InchiKey: UZTJDQYZKQSKGR-UHFFFAOYSA-N
Formula: C12H19ClO2
SMILES: CCC#CC(CC(C)C)OC(=O)CCCl
Mol. weight [g/mol]: 230.73

Physical Properties

Property code	Value	Unit	Source
gf	2.23	kJ/mol	Joback Method
hf	-289.81	kJ/mol	Joback Method
hfus	29.90	kJ/mol	Joback Method
hvap	57.22	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	2.987		Crippen Method
mcvol	191.020	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	1463.00		NIST Webbook
rinpol	1463.00		NIST Webbook
tb	595.80	K	Joback Method
tc	796.63	K	Joback Method
tf	403.18	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.46	J/mol×K	595.80	Joback Method
cpg	473.57	J/mol×K	629.27	Joback Method
cpg	487.94	J/mol×K	662.74	Joback Method
cpg	501.58	J/mol×K	696.22	Joback Method
cpg	514.51	J/mol×K	729.69	Joback Method
cpg	526.73	J/mol×K	763.16	Joback Method
cpg	538.26	J/mol×K	796.63	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=U299216&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