3-Chloropropionic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Inchi: InChI=1S/C14H21ClO2/c1-5-6-12(4)13(8-7-11(2)3)17-14(16)9-10-15/h12-13H,2,5-6,9-10

InchiKey: NOIASPFJFXMZDP-UHFFFAOYSA-N

Formula: C14H21ClO2

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

Mol. weight [g/mol]: 256.77

Physical Properties

Property code	Value	Unit	Source
gf	98.36	kJ/mol	Joback Method
hf	-215.45	kJ/mol	Joback Method
hfus	32.49	kJ/mol	Joback Method
hvap	61.08	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.543		Crippen Method
mcvol	214.900	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
rinpol	1593.00		NIST Webbook
tb	638.12	K	Joback Method
tc	840.24	K	Joback Method
tf	410.00	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.97	J/mol×K	638.12	Joback Method
cpg	553.91	J/mol×K	671.81	Joback Method
cpg	569.01	J/mol×K	705.49	Joback Method
cpg	583.29	J/mol×K	739.18	Joback Method
cpg	596.77	J/mol×K	772.87	Joback Method
cpg	609.47	J/mol×K	806.56	Joback Method
cpg	621.43	J/mol×K	840.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299218&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