3-Chloropropionic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C9H13ClO2/c1-3-5-8(4-2)12-9(11)6-7-10/h8H,4,6-7H2,1-2H3
InchiKey: GEBZZBIUKLVCOU-UHFFFAOYSA-N
Formula: C9H13ClO2
SMILES: CC#CC(CC)OC(=O)CCCl
Mol. weight [g/mol]: 188.65

Physical Properties

Property code	Value	Unit	Source
gf	-20.59	kJ/mol	Joback Method
hf	-222.61	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	50.93	kJ/mol	Joback Method
log10ws	-2.51		Crippen Method
logp	1.960		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1277.00		NIST Webbook
tb	527.60	K	Joback Method
tc	733.26	K	Joback Method
tf	384.37	K	Joback Method
vc	0.569	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.40	J/mol×K	527.60	Joback Method
cpg	329.61	J/mol×K	561.88	Joback Method
cpg	341.28	J/mol×K	596.15	Joback Method
cpg	352.40	J/mol×K	630.43	Joback Method
cpg	362.98	J/mol×K	664.71	Joback Method
cpg	373.02	J/mol×K	698.98	Joback Method
cpg	382.53	J/mol×K	733.26	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299215&Units=SI

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