5-Chlorovaleric acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C11H17ClO2/c1-3-7-10(4-2)14-11(13)8-5-6-9-12/h10H,4-6,8-9H2,1-2H3
InchiKey: PVSFHUUTAKAGCC-UHFFFAOYSA-N
Formula: C11H17ClO2
SMILES: CC#CC(CC)OC(=O)CCCCCl
Mol. weight [g/mol]: 216.70

Physical Properties

Property code	Value	Unit	Source
gf	-3.75	kJ/mol	Joback Method
hf	-263.89	kJ/mol	Joback Method
hfus	30.83	kJ/mol	Joback Method
hvap	55.39	kJ/mol	Joback Method
log10ws	-3.35		Crippen Method
logp	2.741		Crippen Method
mcvol	176.930	ml/mol	McGowan Method
pc	2274.07	kPa	Joback Method
rinpol	1524.50		NIST Webbook
rinpol	1524.50		NIST Webbook
tb	573.36	K	Joback Method
tc	773.06	K	Joback Method
tf	406.91	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.42	J/mol×K	573.36	Joback Method
cpg	423.46	J/mol×K	606.64	Joback Method
cpg	436.84	J/mol×K	639.93	Joback Method
cpg	449.56	J/mol×K	673.21	Joback Method
cpg	461.65	J/mol×K	706.49	Joback Method
cpg	473.11	J/mol×K	739.78	Joback Method
cpg	483.94	J/mol×K	773.06	Joback Method

Sources

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=U292476&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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