5-chlorovaleric acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C9H13ClO2/c1-3-8(2)12-9(11)6-4-5-7-10/h1,8H,4-7H2,2H3
InchiKey: DKDCXIDSBYMDQQ-UHFFFAOYSA-N
Formula: C9H13ClO2
SMILES: C#CC(C)OC(=O)CCCCCl
Mol. weight [g/mol]: 188.65

Physical Properties

Property code	Value	Unit	Source
hf	-328.22	kJ/mol	Cheméo Relay (1.0)
hfus	25.50	kJ/mol	Joback Method
hvap	64.74	kJ/mol	Cheméo Relay (1.0)
ie	10.32	eV	Cheméo Relay (1.0)
logp	1.960		Crippen Method
mcvol	148.750	ml/mol	McGowan Method
rinpol	1291.10		NIST Webbook
tb	472.78	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.47	J/mol×K	508.72	Joback Method
cpg	329.23	J/mol×K	541.22	Joback Method
cpg	340.44	J/mol×K	573.71	Joback Method
cpg	351.11	J/mol×K	606.21	Joback Method
cpg	361.26	J/mol×K	638.70	Joback Method
cpg	370.89	J/mol×K	671.20	Joback Method
cpg	380.02	J/mol×K	703.70	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U292473&Units=SI

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature