Propanoic acid, 3-chloro, 2-propynyl ester

Inchi: InChI=1S/C6H7ClO2/c1-2-5-9-6(8)3-4-7/h1H,3-5H2
InchiKey: YDELXAFUTFIRRH-UHFFFAOYSA-N
Formula: C6H7ClO2
SMILES: C#CCOC(=O)CCCl
Mol. weight [g/mol]: 146.57

Physical Properties

Property code	Value	Unit	Source
gf	-23.14	kJ/mol	Joback Method
hf	-135.81	kJ/mol	Joback Method
hfus	21.26	kJ/mol	Joback Method
hvap	42.35	kJ/mol	Joback Method
log10ws	-1.14		Crippen Method
logp	0.792		Crippen Method
mcvol	106.480	ml/mol	McGowan Method
pc	3731.66	kPa	Joback Method
rinpol	1008.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	998.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1742.00		NIST Webbook
ripol	1723.00		NIST Webbook
tb	440.52	K	Joback Method
tc	638.24	K	Joback Method
tf	306.43	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.50	J/mol×K	440.52	Joback Method

cpg	204.32	J/mol×K	473.47	Joback Method
cpg	211.81	J/mol×K	506.43	Joback Method
cpg	218.96	J/mol×K	539.38	Joback Method
cpg	225.79	J/mol×K	572.33	Joback Method
cpg	232.29	J/mol×K	605.29	Joback Method
cpg	238.48	J/mol×K	638.24	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=R113850&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume