Propanoic acid, 2-chloro, 2-propynyl ester

Other names: prop-2-ynyl-2-chloropropionate
Inchi: InChI=1S/C6H7ClO2/c1-3-4-9-6(8)5(2)7/h1,5H,4H2,2H3
InchiKey: IOJGKOMZXQERIZ-UHFFFAOYSA-N
Formula: C6H7ClO2
SMILES: C#CCOC(=O)C(C)Cl
Mol. weight [g/mol]: 146.57
CAS: 55360-12-8

Physical Properties

Property code	Value	Unit	Source
gf	-25.58	kJ/mol	Joback Method
hf	-141.09	kJ/mol	Joback Method
hfus	17.73	kJ/mol	Joback Method
hvap	41.96	kJ/mol	Joback Method
log10ws	-1.26		Crippen Method
logp	0.790		Crippen Method
mcvol	106.480	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	953.00		NIST Webbook
rinpol	933.00		NIST Webbook
rinpol	914.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	924.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1580.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1575.00		NIST Webbook
tb	440.08	K	Joback Method
tc	642.49	K	Joback Method
tf	291.43	K	Joback Method
vc	0.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	196.65	J/mol×K	440.08	Joback Method
cpg	204.75	J/mol×K	473.81	Joback Method
cpg	212.49	J/mol×K	507.55	Joback Method
cpg	219.87	J/mol×K	541.28	Joback Method
cpg	226.90	J/mol×K	575.02	Joback Method
cpg	233.58	J/mol×K	608.75	Joback Method
cpg	239.92	J/mol×K	642.49	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=C55360128&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