Butanoic acid, 3-chloro, 2-propynyl ester

Inchi: InChI=1S/C7H9ClO2/c1-3-4-10-7(9)5-6(2)8/h1,6H,4-5H2,2H3
InchiKey: SXWQUSUURHRLLH-UHFFFAOYSA-N
Formula: C7H9ClO2
SMILES: C#CCOC(=O)CC(C)Cl
Mol. weight [g/mol]: 160.60

Physical Properties

Property code	Value	Unit	Source
gf	-17.16	kJ/mol	Joback Method
hf	-161.73	kJ/mol	Joback Method
hfus	20.32	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.180		Crippen Method
mcvol	120.570	ml/mol	McGowan Method
pc	3360.64	kPa	Joback Method
rinpol	1045.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1020.00		NIST Webbook
rinpol	1017.00		NIST Webbook
rinpol	1035.00		NIST Webbook
ripol	1797.00		NIST Webbook
ripol	1749.00		NIST Webbook
ripol	1765.00		NIST Webbook
ripol	1749.00		NIST Webbook
tb	462.96	K	Joback Method
tc	662.95	K	Joback Method
tf	302.70	K	Joback Method
vc	0.457	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.78	J/mol×K	462.96	Joback Method

cpg	244.24	J/mol×K	496.29	Joback Method
cpg	253.27	J/mol×K	529.62	Joback Method
cpg	261.88	J/mol×K	562.96	Joback Method
cpg	270.07	J/mol×K	596.29	Joback Method
cpg	277.85	J/mol×K	629.62	Joback Method
cpg	285.23	J/mol×K	662.95	Joback Method

Sources

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=R28796&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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