Butanoic acid, 4-chloro, 2-propynyl ester

Inchi: InChI=1S/C7H9ClO2/c1-2-6-10-7(9)4-3-5-8/h1H,3-6H2
InchiKey: DEICQYWFSRQMEV-UHFFFAOYSA-N
Formula: C7H9ClO2
SMILES: C#CCOC(=O)CCCCl
Mol. weight [g/mol]: 160.60

Physical Properties

Property code	Value	Unit	Source
gf	-14.72	kJ/mol	Joback Method
hf	-156.45	kJ/mol	Joback Method
hfus	23.85	kJ/mol	Joback Method
hvap	44.58	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.182		Crippen Method
mcvol	120.570	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
rinpol	1111.00		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1109.00		NIST Webbook
rinpol	1089.00		NIST Webbook
ripol	1892.00		NIST Webbook
ripol	1867.00		NIST Webbook
ripol	1858.00		NIST Webbook
ripol	1817.00		NIST Webbook
ripol	1817.00		NIST Webbook
tb	463.40	K	Joback Method
tc	658.89	K	Joback Method
tf	317.70	K	Joback Method
vc	0.463	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.58	J/mol×K	463.40	Joback Method

cpg	243.75	J/mol×K	495.98	Joback Method
cpg	252.51	J/mol×K	528.56	Joback Method
cpg	260.88	J/mol×K	561.14	Joback Method
cpg	268.86	J/mol×K	593.73	Joback Method
cpg	276.45	J/mol×K	626.31	Joback Method
cpg	283.67	J/mol×K	658.89	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R28942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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