Ethyl 2-chloro-2-cyanopropanoate

Inchi: InChI=1S/C6H8ClNO2/c1-3-10-5(9)6(2,7)4-8/h3H2,1-2H3
InchiKey: WVSHMLDANLHKIZ-UHFFFAOYSA-N
Formula: C6H8ClNO2
SMILES: CCOC(=O)C(C)(Cl)C#N
Mol. weight [g/mol]: 161.59
CAS: 116374-01-7

Physical Properties

Property code	Value	Unit	Source
gf	-110.19	kJ/mol	Joback Method
hf	-271.58	kJ/mol	Joback Method
hfus	12.37	kJ/mol	Joback Method
hvap	51.67	kJ/mol	Joback Method
log10ws	-1.33		Crippen Method
logp	1.071		Crippen Method
mcvol	116.460	ml/mol	McGowan Method
pc	3117.52	kPa	Joback Method
tb	549.25	K	Joback Method
tc	764.61	K	Joback Method
tf	326.87	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.79	J/mol×K	549.25	Joback Method
cpg	257.39	J/mol×K	585.14	Joback Method
cpg	265.45	J/mol×K	621.04	Joback Method
cpg	272.98	J/mol×K	656.93	Joback Method
cpg	280.02	J/mol×K	692.83	Joback Method
cpg	286.58	J/mol×K	728.72	Joback Method
cpg	292.67	J/mol×K	764.61	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=C116374017&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume