Ethyl 2-cyanopropionate

Other names:	2-Cyanopropionic acid ethyl ester
	Propanoic acid, 2-cyano-, ethyl ester
	Ethyl 2-cyanopropanoate
Inchi:	InChI=1S/C6H9NO2/c1-3-9-6(8)5(2)4-7/h5H,3H2,1-2H3
InchiKey:	MIHRVXYXORIINI-UHFFFAOYSA-N
Formula:	C6H9NO2
SMILES:	CCOC(=O)C(C)C#N
Mol. weight [g/mol]:	127.14
CAS:	1572-99-2

Physical Properties

Property code	Value	Unit	Source
chl	-3276.80 ± 0.29	kJ/mol	NIST Webbook
gf	-103.54	kJ/mol	Joback Method
hf	-311.96 ± 0.63	kJ/mol	NIST Webbook
hfl	-370.54 ± 0.54	kJ/mol	NIST Webbook
hfus	12.07	kJ/mol	Joback Method
hvap	58.58 ± 0.29	kJ/mol	NIST Webbook
hvap	58.60 ± 0.30	kJ/mol	NIST Webbook
log10ws	-0.82		Crippen Method
logp	0.709		Crippen Method
mcvol	104.220	ml/mol	McGowan Method
pc	3210.04	kPa	Joback Method
tb	514.61	K	Joback Method
tc	716.89	K	Joback Method
tf	279.53	K	Joback Method
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	223.62	J/mol×K	514.61	Joback Method
cpg	232.39	J/mol×K	548.32	Joback Method
cpg	240.80	J/mol×K	582.04	Joback Method

cpg	248.83	J/mol×K	615.75	Joback Method
cpg	256.49	J/mol×K	649.47	Joback Method
cpg	263.78	J/mol×K	683.18	Joback Method
cpg	270.68	J/mol×K	716.89	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1572992&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfl: Liquid phase 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