Carbonocyanidic acid, ethyl ester

Other names:	Formic acid, cyano-, ethyl ester
	Ethyl cyanoformate
	C2H5OC(O)CN
	Cyanoformic acid, ethyl ester
	NCCOOC2H5
Inchi:	InChI=1S/C4H5NO2/c1-2-7-4(6)3-5/h2H2,1H3
InchiKey:	MSMGXWFHBSCQFB-UHFFFAOYSA-N
Formula:	C4H5NO2
SMILES:	CCOC(=O)C#N
Mol. weight [g/mol]:	99.09
CAS:	623-49-4

Physical Properties

Property code	Value	Unit	Source
affp	745.70	kJ/mol	NIST Webbook
basg	714.70	kJ/mol	NIST Webbook
gf	-117.94	kJ/mol	Joback Method
hf	-205.81	kJ/mol	Joback Method
hfus	10.41	kJ/mol	Joback Method
hvap	44.13	kJ/mol	Joback Method
log10ws	-0.23		Crippen Method
logp	0.073		Crippen Method
mcvol	76.040	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
rinpol	750.00		NIST Webbook
tb	388.70	K	NIST Webbook
tc	672.61	K	Joback Method
tf	271.99	K	Joback Method
vc	0.309	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.06	J/mol×K	469.29	Joback Method

cpg	150.86	J/mol×K	503.18	Joback Method
cpg	156.48	J/mol×K	537.06	Joback Method
cpg	161.89	J/mol×K	570.95	Joback Method
cpg	167.09	J/mol×K	604.84	Joback Method
cpg	172.07	J/mol×K	638.73	Joback Method
cpg	176.83	J/mol×K	672.61	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=C623494&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume