

Acetic acid, cyano-

Other names:	Cyanoacetic acid
	Malonic mononitrile
	Monocyanoacetic acid
	NCCH2COOH
	2-Cyanoacetic acid
	Acide cyanacetique
	USAF KF-17
	Cyanessigsaeure
	Kyselina kyanoctova
	Cyanoethanoic acid
Inchi:	InChI=1S/C3H3NO2/c4-2-1-3(5)6/h1H2,(H,5,6)
InchiKey:	MLIREBYILWEBDM-UHFFFAOYSA-N
Formula:	C3H3NO2
SMILES:	N#CCC(=O)O
Mol. weight [g/mol]:	85.06
CAS:	372-09-8

Physical Properties

Property code	Value	Unit	Source
chs	-1254.00	kJ/mol	NIST Webbook
gf	-158.18	kJ/mol	Joback Method
hf	-205.18	kJ/mol	Joback Method
hfs	-355.60	kJ/mol	NIST Webbook
hfus	10.72	kJ/mol	Joback Method
hvap	56.17	kJ/mol	Joback Method
log10ws	-0.04		Crippen Method
logp	-0.015		Crippen Method
mcvol	61.950	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
tb	516.17	K	Joback Method
tc	711.31	K	Joback Method
tf	299.31	K	Joback Method
vc	0.255	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	118.93	J/mol×K	516.17	Joback Method
cpg	122.77	J/mol×K	548.69	Joback Method
cpg	126.41	J/mol×K	581.22	Joback Method
cpg	129.87	J/mol×K	613.74	Joback Method
cpg	133.15	J/mol×K	646.26	Joback Method
cpg	136.25	J/mol×K	678.79	Joback Method
cpg	139.19	J/mol×K	711.31	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	381.20	K	0.03	NIST Webbook

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=C372098&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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