Acetic acid, cyano-, methyl ester

Other names:	Cyanoacetic acid methyl ester
	Malonic methyl ester nitrile
	Methyl 2-cyanoacetate
	Methyl cyanoacetate
	Methyl cyanoethanoate
	Methylester kyseliny kyanoctove
	USAF kf-22
Inchi:	InChI=1S/C4H5NO2/c1-7-4(6)2-3-5/h2H2,1H3
InchiKey:	ANGDWNBGPBMQHW-UHFFFAOYSA-N
Formula:	C4H5NO2
SMILES:	COC(=O)CC#N
Mol. weight [g/mol]:	99.09
CAS:	105-34-0

Physical Properties

Property code	Value	Unit	Source
chl	-1979.10 ± 0.46	kJ/mol	NIST Webbook
chl	-1977.00	kJ/mol	NIST Webbook
gf	-117.94	kJ/mol	Joback Method
hf	-243.30 ± 1.10	kJ/mol	NIST Webbook
hfl	-312.00	kJ/mol	NIST Webbook
hfl	-309.53 ± 0.54	kJ/mol	NIST Webbook
hfus	10.41	kJ/mol	Joback Method
hvap	66.20 ± 0.90	kJ/mol	NIST Webbook
hvap	66.23 ± 0.88	kJ/mol	NIST Webbook
hvap	56.20 ± 4.20	kJ/mol	NIST Webbook
ie	10.87 ± 0.05	eV	NIST Webbook
log10ws	-0.23		Crippen Method
logp	0.073		Crippen Method
mcvol	76.040	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
rinpol	900.00		NIST Webbook
rinpol	900.00		NIST Webbook
tb	478.70	K	NIST Webbook
tb	473.70	K	NIST Webbook
tc	672.61	K	Joback Method
tf	260.00 ± 0.02	K	NIST Webbook

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
hvapt	54.90	kJ/mol	479.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.20	K	4.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52851e+01
Coeff. B	-4.35259e+03
Coeff. C	-7.06500e+01
Temperature range (K), min.	360.87
Temperature range (K), max.	507.06

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C105340&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume