Acetamide, 2-cyano-

Other names:	2-cyanoacetamide
	2-cyanoethanamide
	3-Nitrilo-propionamide
	Amid kyseliny kyanoctove
	CAA
	Cyanacetamide
	Cyanoacetamide
	Cyanoiminoacetic acid
	Kyanacetamid
	Malonamide nitrile
	Malonamonitrile
	NSC 6285
	Nitrilomalonamide
	Propionamide, 3-nitrilo-
	USAF KF-14
	ethanamide, 2-cyano-
	«alpha»-Cyanoacetamide
Inchi:	InChI=1S/C3H4N2O/c4-2-1-3(5)6/h1H2,(H2,5,6)
InchiKey:	DGJMPUGMZIKDRO-UHFFFAOYSA-N
Formula:	C3H4N2O
SMILES:	N#CCC(N)=O
Mol. weight [g/mol]:	84.08
CAS:	107-91-5

Physical Properties

Property code	Value	Unit	Source
chs	-1577.00	kJ/mol	NIST Webbook
gf	45.09	kJ/mol	Joback Method
hf	-19.16	kJ/mol	Joback Method
hfs	-175.60	kJ/mol	NIST Webbook
hfus	11.83	kJ/mol	Joback Method
hvap	50.14	kJ/mol	Joback Method
log10ws	-0.15		Crippen Method
logp	-0.615		Crippen Method
mcvol	66.060	ml/mol	McGowan Method
pc	5022.80	kPa	Joback Method
tb	496.52	K	Joback Method

tc	716.36	K	Joback Method
tf	387.30 ± 0.20	K	NIST Webbook
tt	392.84	K	Measurement and Correlation of the Solubility of 2-Cyanoacetamide in 14 Pure Solvents and the Mixing Properties of Solutions
vc	0.265	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	128.52	J/mol×K	496.52	Joback Method
cpg	133.52	J/mol×K	533.16	Joback Method
cpg	138.25	J/mol×K	569.80	Joback Method
cpg	142.72	J/mol×K	606.44	Joback Method
cpg	146.92	J/mol×K	643.08	Joback Method
cpg	150.88	J/mol×K	679.72	Joback Method
cpg	154.58	J/mol×K	716.36	Joback Method
cps	111.10	J/mol×K	300.00	NIST Webbook
hfust	21.70	kJ/mol	387.30	NIST Webbook
hfust	1.20	kJ/mol	346.50	NIST Webbook
hfust	21.70	kJ/mol	387.30	NIST Webbook
hsubt	99.70	kJ/mol	336.50	NIST Webbook
sfust	3.46	J/mol×K	346.50	NIST Webbook
sfust	56.03	J/mol×K	387.30	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=C107915&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Correlation of the Solubility of 2-Cyanoacetamide in 14 Pure Solvents and the Mixing Properties of Solutions:	https://www.doi.org/10.1021/acs.jced.8b01205

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase 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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume