

# Acetamide, 2-cyano-

<b>Other names:</b>	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
<b>Inchi:</b>	InChI=1S/C3H4N2O/c4-2-1-3(5)6/h1H2,(H2,5,6)
<b>InchiKey:</b>	DGJMPUGMZIKDRO-UHFFFAOYSA-N
<b>Formula:</b>	C3H4N2O
<b>SMILES:</b>	N#CCC(N)=O
<b>Mol. weight [g/mol]:</b>	84.08
<b>CAS:</b>	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	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	150.88	J/mol×K	679.72	Joback Method
cpg	146.92	J/mol×K	643.08	Joback Method
cpg	154.58	J/mol×K	716.36	Joback Method
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
cps	111.10	J/mol×K	300.00	NIST Webbook
hfust	21.70	kJ/mol	387.30	NIST Webbook
hfust	21.70	kJ/mol	387.30	NIST Webbook
hfust	1.20	kJ/mol	346.50	NIST Webbook
hsubt	99.70	kJ/mol	336.50	NIST Webbook
sfust	56.03	J/mol×K	387.30	NIST Webbook
sfust	3.46	J/mol×K	346.50	NIST Webbook

## Sources

Measurement and Correlation of the Solubility of 2-Cyanoacetamide in 14 Pure Solvents and the Mixing Properties of Solutions: McGowan Method:

<https://www.doi.org/10.1021/acs.jced.8b01205>

NIST Webbook:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

Crippen Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C107915&Units=SI>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

# Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>cps:</b>	Solid phase heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>sfust:</b>	Entropy of fusion at a given temperature
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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