

# 2-Butynedinitrile

<b>Other names:</b>	Acetylenedicarbonitrile Dicyanoacetylene 1,2-Dicyanoacetylene NCC«equiv»CCN Dicyanoethyne Sous-azote de carbone C4N2
<b>Inchi:</b>	InChI=1S/C4N2/c5-3-1-2-4-6
<b>InchiKey:</b>	ZEHZNAXXOOYTJM-UHFFFAOYSA-N
<b>Formula:</b>	C4N2
<b>SMILES:</b>	N#CC#CC#N
<b>Mol. weight [g/mol]:</b>	76.06
<b>CAS:</b>	1071-98-3

## Physical Properties

Property code	Value	Unit	Source
chl	-2074.40 ± 1.30	kJ/mol	NIST Webbook
chs	-2156.00	kJ/mol	NIST Webbook
gf	451.96	kJ/mol	Joback Method
hf	529.30	kJ/mol	NIST Webbook
hfl	500.40	kJ/mol	NIST Webbook
hfus	12.25	kJ/mol	Joback Method
hsub	44.25	kJ/mol	NIST Webbook
hvap	28.90	kJ/mol	NIST Webbook
ie	11.81 ± 0.02	eV	NIST Webbook
ie	11.81 ± 0.01	eV	NIST Webbook
ie	11.40 ± 0.20	eV	NIST Webbook
ie	11.84	eV	NIST Webbook
ie	11.84	eV	NIST Webbook
log10ws	-1.02		Crippen Method
logp	0.037		Crippen Method
mcvol	61.380	ml/mol	McGowan Method
pc	4492.23	kPa	Joback Method
tb	349.70	K	NIST Webbook
tc	749.07	K	Joback Method
tf	370.92	K	Joback Method
vc	0.274	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.11	J/mol×K	667.41	Joback Method
cpg	105.28	J/mol×K	708.24	Joback Method
cpg	93.31	J/mol×K	504.08	Joback Method
cpg	95.94	J/mol×K	544.91	Joback Method
cpg	98.44	J/mol×K	585.74	Joback Method
cpg	100.84	J/mol×K	626.58	Joback Method
cpg	107.33	J/mol×K	749.07	Joback Method
hsubt	44.30	kJ/mol	268.00	NIST Webbook
hvapt	27.30	kJ/mol	322.50	NIST Webbook

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/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=C1071983&Units=SI>

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

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

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>chs:</b>	Standard solid enthalpy of combustion
<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hsub:</b>	Enthalpy of sublimation at standard conditions
<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature

<b>ie:</b>	Ionization energy
<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>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/37-186-5/2-Butynedinitrile.pdf>

Generated by Cheméo on 2024-04-10 18:23:03.389257707 +0000 UTC m=+15062632.309835028.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.