2-Butynedinitrile

Other names:	Acetylenedicarbonitrile
	Dicyanoacetylene
	1,2-Dicyanoacetylene
	NCC«equiv»CCN
	Dicyanoethyne
	Sous-azote de carbone
	C4N2
Inchi:	InChI=1S/C4N2/c5-3-1-2-4-6
InchiKey:	ZEHZNAXXOOYTJM-UHFFFAOYSA-N
Formula:	C4N2
SMILES:	N#CC#CC#N
Mol. weight [g/mol]:	76.06
CAS:	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	11.84	eV	NIST Webbook
ie	11.81 ± 0.02	eV	NIST Webbook
ie	11.81 ± 0.01	eV	NIST Webbook
ie	11.84	eV	NIST Webbook
ie	11.40 ± 0.20	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	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	103.11	J/mol×K	667.41	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
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/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid enthalpy of combustion
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
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume