Propiolonitrile

Other names:	2-Propynenitrile
	Cyanaethylene
	Cyanoacetylene
	Cyanoethyne
	HC«equiv»CCN
	HCÂ«equivÂ»CCN
	Propynenitrile
Inchi:	InChI=1S/C3HN/c1-2-3-4/h1H
InchiKey:	LNDJVIYUJOJFSO-UHFFFAOYSA-N
Formula:	C3HN
SMILES:	C#CC#N
Mol. weight [g/mol]:	51.05
CAS:	1070-71-9

Physical Properties

Property code	Value	Unit	Source
affp	751.20	kJ/mol	NIST Webbook
basg	720.50	kJ/mol	NIST Webbook
ea	1.04 ± 0.05	eV	NIST Webbook
ea	2.56 ± 0.22	eV	NIST Webbook
gf	330.63	kJ/mol	Joback Method
hf	354.00	kJ/mol	NIST Webbook
hfus	8.01	kJ/mol	Joback Method
hvap	32.61	kJ/mol	Joback Method
ie	11.62 ± 0.03	eV	NIST Webbook
ie	11.60 ± 0.01	eV	NIST Webbook
ie	11.60 ± 0.20	eV	NIST Webbook
ie	11.75	eV	NIST Webbook
ie	11.56 ± 0.04	eV	NIST Webbook
ie	11.64 ± 0.01	eV	NIST Webbook
ie	11.60	eV	NIST Webbook
log10ws	-0.74		Crippen Method
logp	0.143		Crippen Method
mcvol	45.910	ml/mol	McGowan Method
pc	5228.24	kPa	Joback Method
rinpol	424.00		NIST Webbook
rinpol	447.60		NIST Webbook

rinpol	447.60		NIST Webbook
rinpol	421.00		NIST Webbook
tb	315.70	K	NIST Webbook
tc	568.69	K	Joback Method
tf	235.53	K	Joback Method
vc	0.192	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	65.83	J/mol×K	360.24	Joback Method
cpg	68.15	J/mol×K	394.98	Joback Method
cpg	70.31	J/mol×K	429.72	Joback Method
cpg	72.34	J/mol×K	464.47	Joback Method
cpg	74.24	J/mol×K	499.21	Joback Method
cpg	76.02	J/mol×K	533.95	Joback Method
cpg	77.69	J/mol×K	568.69	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.23002e+01
Coeff. B	-1.64157e+03
Coeff. C	-1.02005e+02
Temperature range (K), min.	238.66
Temperature range (K), max.	336.89

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=C1070719&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

Legend

affp:	Proton affinity
basg:	Gas basicity
cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume