

Cyanopropyne

Other names:	CH ₃ C«equiv»CCN Prop-1-yne, 1-cyano-
Inchi:	InChI=1S/C4H3N/c1-2-3-4-5/h1H3
InchiKey:	WNXDCVVDPKHWMW-UHFFFAOYSA-N
Formula:	C ₄ H ₃ N
SMILES:	CC#CC#N
Mol. weight [g/mol]:	65.07
CAS:	13752-78-8

Physical Properties

Property code	Value	Unit	Source
gf	318.78	kJ/mol	Joback Method
hf	311.29	kJ/mol	Joback Method
hfus	10.74	kJ/mol	Joback Method
hvap	37.13	kJ/mol	Joback Method
ie	10.95	eV	NIST Webbook
ie	10.78 ± 0.02	eV	NIST Webbook
log10ws	-1.16		Crippen Method
logp	0.533		Crippen Method
mcvol	60.000	ml/mol	McGowan Method
pc	4646.65	kPa	Joback Method
rinpol	637.90		NIST Webbook
rinpol	595.00		NIST Webbook
rinpol	596.00		NIST Webbook
rinpol	637.90		NIST Webbook
tb	402.00	K	Joback Method
tc	623.50	K	Joback Method
tf	305.93	K	Joback Method
vc	0.247	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	90.85	J/mol×K	402.00	Joback Method

cpg	95.06	J/mol×K	438.92	Joback Method
cpg	99.12	J/mol×K	475.83	Joback Method
cpg	103.02	J/mol×K	512.75	Joback Method
cpg	106.76	J/mol×K	549.67	Joback Method
cpg	110.36	J/mol×K	586.58	Joback Method
cpg	113.80	J/mol×K	623.50	Joback Method

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=C13752788&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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