Cyclopropanecarbonitrile

Other names:	Cyanocyclopropane
	Cyclopropanecarboxylic acid nitrile
	Cyclopropanenitrile
	Cyclopropylnitrile
	cyclopropyl cyanide
Inchi:	InChI=1S/C4H5N/c5-3-4-1-2-4/h4H,1-2H2
InchiKey:	AUQDITHEDVOTCU-UHFFFAOYSA-N
Formula:	C4H5N
SMILES:	N#CC1CC1
Mol. weight [g/mol]:	67.09
CAS:	5500-21-0

Physical Properties

Property code	Value	Unit	Source
affp	808.20	kJ/mol	NIST Webbook
basg	777.50	kJ/mol	NIST Webbook
chl	-2433.00	kJ/mol	NIST Webbook
chl	-2429.40 ± 0.71	kJ/mol	NIST Webbook
gf	176.73	kJ/mol	Joback Method
hf	180.60	kJ/mol	NIST Webbook
hf	182.70 ± 0.70	kJ/mol	NIST Webbook
hfl	140.80	kJ/mol	NIST Webbook
hfus	5.76	kJ/mol	Joback Method
hvap	39.80 ± 0.40	kJ/mol	NIST Webbook
hvap	41.90 ± 0.10	kJ/mol	NIST Webbook
hvap	41.94 ± 0.11	kJ/mol	NIST Webbook
hvap	39.80	kJ/mol	NIST Webbook
hvap	39.80	kJ/mol	NIST Webbook
hvap	41.97	kJ/mol	NIST Webbook
ie	10.25	eV	NIST Webbook
ie	11.20 ± 0.20	eV	NIST Webbook
log10ws	-1.02		Crippen Method
logp	0.920		Crippen Method
mcvol	57.740	ml/mol	McGowan Method
pc	4462.28	kPa	Joback Method
rinpol	644.00		NIST Webbook
rinpol	684.00		NIST Webbook

rinpol	684.00		NIST Webbook
rinpol	645.00		NIST Webbook
tb	404.90 ± 3.00	K	NIST Webbook
tb	408.20	K	NIST Webbook
tb	407.50 ± 0.50	K	NIST Webbook
tb	408.20	K	NIST Webbook
tc	609.13	K	Joback Method
tf	217.77	K	Joback Method
vc	0.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	100.75	J/mol×K	399.74	Joback Method
cpg	108.34	J/mol×K	434.64	Joback Method
cpg	115.41	J/mol×K	469.54	Joback Method
cpg	122.00	J/mol×K	504.44	Joback Method
cpg	128.12	J/mol×K	539.33	Joback Method
cpg	133.82	J/mol×K	574.23	Joback Method
cpg	139.13	J/mol×K	609.13	Joback Method
cpl	115.40	J/mol×K	297.00	NIST Webbook
hvapt	35.55	kJ/mol	408.20	NIST Webbook
hvapt	39.40	kJ/mol	350.50	NIST Webbook
pvap	35.20	kPa	373.10	Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane + trans-1,2-Dichloroethylene, 1-Octene + 2-Methyl Thiophene, 2-Ethyl Thiophene + 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile + Water

pvap	102.20	kPa	408.15	Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane + trans-1,2-Dichloroethylene, 1-Octene + 2-Methyl Thiophene, 2-Ethyl Thiophene + 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile + Water

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5500210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase Equilibria on Four Binary Systems: 1,2-Dichloroethane + trans-1,2-Dichloroethylene, 1-Octene + 2-Methyl Thiophene, 2-Ethyl Thiophene + 2,2,4-Trimethylpentane, and Cyclopropanecarbonitrile + Water:	https://www.doi.org/10.1021/je050473r
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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

pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume