Cyclohexanecarbonitrile

Other names:	Cyanocyclohexane
	Cyclohexanecarboxylic acid nitrile
	Cyclohexyl cyanide
	Hexahydrobenzonitrile
Inchi:	InChI=1S/C7H11N/c8-6-7-4-2-1-3-5-7/h7H,1-5H2
InchiKey:	VBWIZSYFQSOUFQ-UHFFFAOYSA-N
Formula:	C7H11N
SMILES:	N#CC1CCCCC1
Mol. weight [g/mol]:	109.17
CAS:	766-05-2

Physical Properties

Property code	Value	Unit	Source
affp	815.00	kJ/mol	NIST Webbook
basg	784.40	kJ/mol	NIST Webbook
chl	-4267.60 ± 2.30	kJ/mol	NIST Webbook
chl	-4279.48 ± 0.50	kJ/mol	NIST Webbook
gf	165.69	kJ/mol	Joback Method
hf	-3.60	kJ/mol	NIST Webbook
hf	-7.24	kJ/mol	NIST Webbook
hfl	-59.12	kJ/mol	NIST Webbook
hfl	-47.20	kJ/mol	NIST Webbook
hfus	7.23	kJ/mol	Joback Method
hvap	42.08	kJ/mol	Joback Method
log10ws	-2.27		Crippen Method
logp	2.090		Crippen Method
mcvol	100.010	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
tb	461.40 ± 0.20	K	NIST Webbook
tc	708.27	K	Joback Method
tf	285.20 ± 0.20	K	NIST Webbook
vc	0.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.20	J/mol×K	632.58	Joback Method
cpg	274.23	J/mol×K	670.42	Joback Method
cpg	211.28	J/mol×K	481.19	Joback Method
cpg	225.48	J/mol×K	519.04	Joback Method
cpg	238.85	J/mol×K	556.88	Joback Method
cpg	251.42	J/mol×K	594.73	Joback Method
cpg	284.53	J/mol×K	708.27	Joback Method
cpl	177.90	J/mol×K	297.00	NIST Webbook
hfust	7.43	kJ/mol	215.00	NIST Webbook
hfust	3.64	kJ/mol	285.10	NIST Webbook
hfust	3.64	kJ/mol	285.10	NIST Webbook
hvapt	39.40	kJ/mol	380.00	NIST Webbook
sfust	12.75	J/mol×K	285.10	NIST Webbook
sfust	34.53	J/mol×K	215.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	355.00 ± 2.00	K	2.40	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C766052&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume