3-Pyridinecarbonitrile

Other names:	3-Azabenzonitrile
	3-Cyjanopirydyna
	3-Pyridinenitrile
	3-Pyridyl cyanide
	3-cyanopyridine
	3-pyridylcarbonitrile
	NSC 17558
	Nitryl kwasu nikotynowego
	Pyridine-3-carbonitrile
	nicotinic acid nitrile
	nicotinonitrile
Inchi:	InChI=1S/C6H4N2/c7-4-6-2-1-3-8-5-6/h1-3,5H
InchiKey:	GZPHSAQLYPIAIN-UHFFFAOYSA-N
Formula:	C6H4N2
SMILES:	N#Cc1cccnc1
Mol. weight [g/mol]:	104.11
CAS:	100-54-9

Physical Properties

Property code	Value	Unit	Source
affp	877.00	kJ/mol	NIST Webbook
basg	845.10	kJ/mol	NIST Webbook
chs	-3138.50 ± 0.50	kJ/mol	NIST Webbook
chs	-3126.00	kJ/mol	NIST Webbook
hf	265.40	kJ/mol	NIST Webbook
hf	277.90 ± 2.00	kJ/mol	NIST Webbook
hfs	193.30	kJ/mol	NIST Webbook
hfs	205.80 ± 0.90	kJ/mol	NIST Webbook
hsub	72.10 ± 1.80	kJ/mol	NIST Webbook
hsub	72.10 ± 1.80	kJ/mol	NIST Webbook
hsub	72.10	kJ/mol	NIST Webbook
ie	10.40 ± 0.10	eV	NIST Webbook
ie	10.10	eV	NIST Webbook
ie	10.37	eV	NIST Webbook
log10ws	-1.59		Crippen Method
logp	0.953		Crippen Method
mcvol	83.000	ml/mol	McGowan Method

rinpol	1012.00		NIST Webbook
rinpol	1012.70		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1012.70		NIST Webbook
rinpol	1007.00		NIST Webbook
rinpol	1012.00		NIST Webbook
ripol	1875.00		NIST Webbook
tb	474.00 ± 1.00	K	NIST Webbook
tb	474.20	K	NIST Webbook
tb	515.70	K	NIST Webbook
tb	479.85 ± 0.60	K	NIST Webbook
tf	323.65 ± 1.00	K	NIST Webbook
tf	323.15 ± 1.00	K	NIST Webbook
tf	325.05	K	Measurement and Correlation of Solubility of Two Isomers of Cyanopyridine in Eight Pure Solvents from 268.15 K to 318.15 K

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	45.00	kJ/mol	466.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Measurement and Correlation of Solubility of Two Isomers of Cyanopyridine in Eight Pure Solvents from 268.15 K to 318.15 K:	https://www.doi.org/10.1021/acs.jced.7b00301
Solubility in Different Solvents, Crystal Polymorph and Morphology, and Optimization of Crystallization Process of AIBN:	https://www.doi.org/10.1021/acs.jced.7b00538
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100549&Units=SI

Legend

affp: Proton affinity

basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point