

2-Pyridinecarbonitrile

Other names:	Picolinonitrile Picolinic acid nitrile 2-Cyanopyridine 2-Pyridyl nitrile Pyridine-2-carbonitrile
Inchi:	InChI=1S/C6H4N2/c7-5-6-3-1-2-4-8-6/h1-4H
InchiKey:	FFNVQNRYPFDDP-UHFFFAOYSA-N
Formula:	C6H4N2
SMILES:	N#Cc1ccccn1
Mol. weight [g/mol]:	104.11
CAS:	100-70-9

Physical Properties

Property code	Value	Unit	Source
affp	872.90	kJ/mol	NIST Webbook
basg	841.00	kJ/mol	NIST Webbook
chs	-3142.70 ± 0.50	kJ/mol	NIST Webbook
hf	280.70 ± 1.50	kJ/mol	NIST Webbook
hfs	210.00 ± 0.90	kJ/mol	NIST Webbook
hsub	70.70 ± 1.20	kJ/mol	NIST Webbook
hsub	70.70	kJ/mol	NIST Webbook
hsub	70.70 ± 1.20	kJ/mol	NIST Webbook
ie	10.12	eV	NIST Webbook
ie	10.33	eV	NIST Webbook
ie	10.33 ± 0.05	eV	NIST Webbook
ie	10.50 ± 0.10	eV	NIST Webbook
log10ws	-1.59		Crippen Method
logp	0.953		Crippen Method
mcvol	83.000	ml/mol	McGowan Method
rinpol	1079.00		NIST Webbook
rinpol	1069.00		NIST Webbook
tb	497.70	K	NIST Webbook
tb	486.70	K	NIST Webbook
tb	486.50 ± 1.50	K	NIST Webbook
tf	302.15 ± 2.00	K	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C100709&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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