4-Pyridinecarboxaldehyde

Other names:	Isonicotinaldehyde
	p-Pyridinealdehyde
	Isonicotinic aldehyde
	Pyridine-4-carbaldehyde
	4-Formylpyridine
	4-Pyridinealdehyde
	Pyridine-4-aldehyde
	Pyridine-4-carboxaldehyde
	4-Pyridylaldehyde
	4-Pyridinecarbaldehyde
	NSC 8953
	p-Formylpyridine
Inchi:	InChI=1S/C6H5NO/c8-5-6-1-3-7-4-2-6/h1-5H
InchiKey:	BGUWFUQJCDRPTL-UHFFFAOYSA-N
Formula:	C6H5NO
SMILES:	O=Cc1ccncc1
Mol. weight [g/mol]:	107.11
CAS:	872-85-5

Physical Properties

Property code	Value	Unit	Source
affp	904.60	kJ/mol	NIST Webbook
basg	872.80	kJ/mol	NIST Webbook
ie	10.12 ± 0.05	eV	NIST Webbook
log10ws	-1.48		Crippen Method
logp	0.894		Crippen Method
mcvol	83.190	ml/mol	McGowan Method
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1668.00		NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.70	K	1.60	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C872855&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tbrp:	Boiling point at reduced pressure