2-Pyridinecarboxaldehyde

Other names:	Picolinaldehyde
	2-Pyridinealdehyde
	Pyridine-2-carboxaldehyde
	Pyridine-2-aldehyde
	2-Pyridylaldehyde
	2-Pyridinecarbaldehyde
	«alpha»-Picolinaldehyde
	o-Nicotinaldehyde
	Picolinal
	Picolinic aldehyde
	2-Formylpyridine
	2-Picolinaldehyde
	2-Picolinealdehyde
	2-Pyridaldehyde
	2-Pyridylcarboxaldehyde
	NSC 8951
	pyridine-2-carbaldehyde
Inchi:	InChI=1S/C6H5NO/c8-5-6-3-1-2-4-7-6/h1-5H
InchiKey:	CSDSSGBPEUDDEE-UHFFFAOYSA-N
Formula:	C6H5NO
SMILES:	O=Cc1ccccn1
Mol. weight [g/mol]:	107.11
CAS:	1121-60-4

Physical Properties

Property code	Value	Unit	Source
ie	9.75 ± 0.05	eV	NIST Webbook
log10ws	-1.48		Crippen Method
logp	0.894		Crippen Method
mcvol	83.190	ml/mol	McGowan Method
rinpol	968.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	968.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1570.00		NIST Webbook
tb	454.20	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	335.70	K	1.70	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=C1121604&Units=SI

Legend

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
tbrp:	Boiling point at reduced pressure