4-Pyridine carboxaldehyde

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

Physical Properties

Property code	Value	Unit	Source
af	0.3838		Cheméo Relay (1.0)
affp	904.60	kJ/mol	NIST Webbook
basg	872.80	kJ/mol	NIST Webbook
gf	57.60	kJ/mol	Cheméo Relay (1.0, beta)
hf	12.90	kJ/mol	Cheméo Relay (1.0)
hvap	57.04	kJ/mol	Cheméo Relay (1.0)
ie	10.12 ± 0.05	eV	NIST Webbook
log10ws	0.20		Cheméo Relay (1.0)
logp	0.894		Crippen Method
mcvol	83.190	ml/mol	McGowan Method
pc	5476.06	kPa	Cheméo Relay (1.0, beta)
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
ripol	1668.00		NIST Webbook
ripol	1668.00		NIST Webbook
tb	468.73	K	Cheméo Relay (1.0)
tc	741.02	K	Cheméo Relay (1.0)

tf	334.34	K	Cheméo Relay (1.0)

Pressure Dependent Properties

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

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C872855&Units=SI

Legend

af: Acentric Factor
affp: Proton affinity
basg: Gas basicity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point