2-PYRIDINECARBOXYLIC ACID

Other names:	Picolinic acid
	«alpha»-Pyridinecarboxylic acid
	o-Pyridinecarboxylic acid
	2-Carboxypyridine
	2-Picolinic acid
	Pyridinecarboxylic acid-(2)
	Acide picolique
	Pyridine-carboxylique-2
	NSC 171
	pyridine-2-carboxylic acid
Inchi:	InChI=1S/C6H5NO2/c8-6(9)5-3-1-2-4-7-5/h1-4H,(H,8,9)
InchiKey:	SIOXPEMLGUPBBT-UHFFFAOYSA-N
Formula:	C6H5NO2
SMILES:	O=C(O)c1ccccn1
Mol. weight [g/mol]:	123.11

Physical Properties

Property code	Value	Unit	Source
af	0.6439		Cheméo Relay (1.0)
chs	-2376.80	kJ/mol	NIST Webbook
gf	-135.77	kJ/mol	Cheméo Relay (1.0, beta)
hf	-237.45	kJ/mol	Cheméo Relay (1.0)
hfs	-343.80 ± 1.80	kJ/mol	NIST Webbook
hsub	92.70 ± 0.50	kJ/mol	NIST Webbook
hsub	98.00 ± 2.30	kJ/mol	NIST Webbook
hvap	77.26	kJ/mol	Cheméo Relay (1.0)
ie	9.33	eV	Cheméo Relay (1.0)
log10ws	-0.41		Cheméo Relay (1.0)
logp	0.780		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	5204.24	kPa	Cheméo Relay (1.0, beta)
tb	537.97	K	Cheméo Relay (1.0)
tc	787.23	K	Cheméo Relay (1.0)
tf	395.58	K	Cheméo Relay (1.0)
vc	0.318	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	30.00	kJ/mol	411.00	NIST Webbook
hfust	30.00	kJ/mol	411.00	NIST Webbook
hfust	30.00	kJ/mol	411.00	NIST Webbook
hsubt	91.00 ± 0.50	kJ/mol	329.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C98986&Units=SI
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):

Legend

af: Acentric Factor
chs: Standard solid enthalpy of combustion
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfust: Enthalpy of fusion at a given temperature
hsub: Enthalpy of sublimation at standard conditions
hsubt: Enthalpy of sublimation at a given temperature
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume