3-Pyridinecarboxylic acid, 1,2-dihydro-2-oxo-

Other names: 2-Hydroxynicotinic acid

                      1,2-dihydro-2-oxonicotinic acid

Inchi: InChI=1S/C6H5NO3/c8-5-4(6(9)10)2-1-3-7-5/h1-3H,(H,7,8)(H,9,10)

InchiKey: UEYQJQVBUVAELZ-UHFFFAOYSA-N

Formula: C6H5NO3

SMILES: O=C(O)c1cccnc1O

Mol. weight [g/mol]:   139.11

CAS: 609-71-2

Physical Properties

Property code	Value	Unit	Source
hsub	128.30 ± 5.10	kJ/mol	NIST Webbook
log10ws	-0.85		Crippen Method
logp	0.485		Crippen Method
mcvol	94.930	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	125.40 ± 5.00	kJ/mol	447.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C609712&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

hsub: Enthalpy of sublimation at standard conditions

hsubt: Enthalpy of sublimation at a given temperature

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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