

3-Pyridinecarboxylic acid, 1,6-dihydro-6-oxo-

Other names:	Nicotinic acid, 1,6-dihydro-6-oxo- 1,6-Dihydro-6-oxo-3-pyridinecarboxylic acid 2-Pyridone-5-carboxylic acid 6-Hydroxynicotinic acid 2-Hydroxypyridine-3-carboxylic acid Pyridin-2-one-5-carboxylic acid
Inchi:	InChI=1S/C6H5NO3/c8-5-2-1-4(3-7-5)6(9)10/h1-3H,(H,7,8)(H,9,10)
InchiKey:	BLHCMGRVFXRYRN-UHFFFAOYSA-N
Formula:	C6H5NO3
SMILES:	O=C(O)c1ccc(O)nc1
Mol. weight [g/mol]:	139.11
CAS:	5006-66-6

Physical Properties

Property code	Value	Unit	Source
hsub	146.40 ± 4.60	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	143.00 ± 4.50	kJ/mol	474.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5006666&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.cheméo.com/cid/96-885-4/3-Pyridinecarboxylic-acid-1-6-dihydro-6-oxo.pdf>

Generated by Cheméo on 2024-04-18 07:10:12.381477654 +0000 UTC m=+15713461.302054966.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.