

3-Pyridinecarboxylic acid, 4-hydroxy-

Other names:	4-hydroxynicotinic acid
Inchi:	InChI=1S/C6H5NO3/c8-5-1-2-7-3-4(5)6(9)10/h1-3H,(H,7,8)(H,9,10)
InchiKey:	CHCUBGPSZDGABM-UHFFFAOYSA-N
Formula:	C6H5NO3
SMILES:	O=C(O)c1c[nH]ccc1=O
Mol. weight [g/mol]:	139.11
CAS:	609-70-1

Physical Properties

Property code	Value	Unit	Source
hsub	148.10 ± 3.70	kJ/mol	NIST Webbook
log10ws	-0.17		Crippen Method
logp	-0.409		Crippen Method
mvol	94.930	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	144.60 ± 3.60	kJ/mol	440.50	NIST Webbook

Sources

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=C609701&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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