

4-Pyridinecarboxylic acid

Other names:	4-Picolinic acid 4-carboxypyridine Acide iso-nicotinique INA Pyridine-4-carboxylic acid Pyridinecarboxylic acid-(4) isonicotinic acid «alpha»-Picolinic acid «gamma»-Picolinic acid
Inchi:	InChI=1S/C6H5NO2/c8-6(9)5-1-3-7-4-2-5/h1-4H,(H,8,9)
InchiKey:	TWBYWOBDOCUKOW-UHFFFAOYSA-N
Formula:	C6H5NO2
SMILES:	O=C(O)c1ccncc1
Mol. weight [g/mol]:	123.11
CAS:	55-22-1

Physical Properties

Property code	Value	Unit	Source
hsub	111.30 ± 0.60	kJ/mol	NIST Webbook
hsub	113.90 ± 4.70	kJ/mol	NIST Webbook
log10ws	-1.30		Crippen Method
logp	0.780		Crippen Method
mvol	89.060	ml/mol	McGowan Method
ripol	2088.00		NIST Webbook
tf	590.65 ± 1.00	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	135.00	kJ/mol	593.00	NIST Webbook
hfust	135.00	kJ/mol	593.00	NIST Webbook
hfust	135.00	kJ/mol	593.00	NIST Webbook
hsubt	107.70 ± 0.70	kJ/mol	362.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55221&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
On the solubility of nicotinic acid and isonicotinic acid in water and organic solvents	https://www.doi.org/10.1016/j.jct.2013.01.024
Solubility of Isonicotinic Acid in 4-Methylpyridine + Water from (287.65 to 361.45) K	https://www.doi.org/10.1021/je800352u
Solubility of Isonicotinic Acid in (Methanol, Ethanol, 1-Propanol, 2-Propanol, and 1,2-Propanediol)	https://www.doi.org/10.1021/je800824h
Solubility of Nicotinic Acid in Ethyl Acetate + Water from (289.65 to 358.75) K	https://www.doi.org/10.1021/je900871q
McGowan Method: Sulfuric Acid + Water from (293.55 to 361.45) K:	http://link.springer.com/article/10.1007/BF02311772

Legend

hfust:	Enthalpy of fusion at a given temperature
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
ripol:	Polar retention indices
tf:	Normal melting (fusion) point

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