

4-Pyridinecarboxamide

Other names:	.gamma.-pyridinecarboxamide 4-carbamoylpyridine Pyridine-4-carboxylic acid amide isonicotinamide isonicotinic acid amide «gamma»-Pyridinecarboxamide
Inchi:	InChI=1S/C6H6N2O/c7-6(9)5-1-3-8-4-2-5/h1-4H,(H2,7,9)
InchiKey:	VFQXVTODMYMSMJ-UHFFFAOYSA-N
Formula:	C6H6N2O
SMILES:	NC(=O)c1ccncc1
Mol. weight [g/mol]:	122.12
CAS:	1453-82-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.41		Crippen Method
logp	0.181		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
tf	428.50	K	Determination and correlation of solubility and mixing properties of isonicotinamide (form II) in some pure solvents

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Determination and correlation of solubility and mixing properties of isonicotinamide (form II) in some pure solvents: Self-Interactions of Isonicotinamide and Isonicotinamide in (Dimethylformamide + Water) and (Dimethylsulfoxide + Water) Mixed Solvents at 298.15 K:	https://www.doi.org/10.1016/j.tca.2016.01.012 https://www.doi.org/10.1021/je500447r http://link.springer.com/article/10.1007/BF02311772 http://webbook.nist.gov/cgi/cbook.cgi?ID=C1453823&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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