Picolinamide

Other names:	Pyridine-2-carboxamide
	«alpha»-Picolinamide
	2-Pyridinecarboxamide
	«alpha»-Picolinic acid amide
	Picolinic acid amide
	Picolinoylamide
	2-Carbamoylpyridine
	Pyridine-2-carboxylicamide
Inchi:	InChI=1S/C6H6N2O/c7-6(9)5-3-1-2-4-8-5/h1-4H,(H2,7,9)
InchiKey:	IBBMAWULFFBRKK-UHFFFAOYSA-N
Formula:	C6H6N2O
SMILES:	NC(=O)c1ccccn1
Mol. weight [g/mol]:	122.12
CAS:	1452-77-3

Physical Properties

Property code	Value	Unit	Source
hsub	93.10 ± 3.30	kJ/mol	NIST Webbook
log10ws	-1.41		Crippen Method
logp	0.181		Crippen Method
mcvol	93.170	ml/mol	McGowan Method
rinpol	1268.00		NIST Webbook
ripol	2358.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	16.82	kJ/mol	381.00	NIST Webbook
hsubt	93.10	kJ/mol	348.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1452773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices