

2-Fluoropyridine

Other names:	Pyridine, 2-fluoro-
Inchi:	InChI=1S/C5H4FN/c6-5-3-1-2-4-7-5/h1-4H
InchiKey:	MTAODLNXYIKSO-UHFFFAOYSA-N
Formula:	C5H4FN
SMILES:	Fc1ccccn1
Mol. weight [g/mol]:	97.09
CAS:	372-48-5

Physical Properties

Property code	Value	Unit	Source
affp	884.60	kJ/mol	NIST Webbook
basg	852.70	kJ/mol	NIST Webbook
ie	9.40	eV	NIST Webbook
log10ws	-1.57		Crippen Method
logp	1.221		Crippen Method
mcvol	69.300	ml/mol	McGowan Method
tb	398.20	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.20	K	100.00	NIST Webbook
tbrp	399.00	K	100.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C372485&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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