

PYRIDINE, 2-FLUORO-

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

Physical Properties

Property code	Value	Unit	Source
af	0.2506		Cheméo Relay (1.0)
gf	5.37	kJ/mol	Cheméo Relay (1.0, beta)
hf	-107.11	kJ/mol	Cheméo Relay (1.0)
hvap	41.39	kJ/mol	Cheméo Relay (1.0)
ie	9.69	eV	Cheméo Relay (1.0)
log10ws	0.26		Cheméo Relay (1.0)
logp	1.221		Crippen Method
mcvol	69.300	ml/mol	McGowan Method
pc	5114.69	kPa	Cheméo Relay (1.0, beta)
tb	383.72	K	Cheméo Relay (1.0)
tc	601.26	K	Cheméo Relay (1.0)
tf	253.80	K	Cheméo Relay (1.0)
vc	0.250	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C372485&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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