

C6H6FN

Inchi:	InChI=1S/C6H6FN/c1-5-2-3-8-6(7)4-5/h2-4H,1H3
InchiKey:	ZBFAXMKJADVOGH-UHFFFAOYSA-N
Formula:	C6H6FN
SMILES:	Cc1ccnc(F)c1
Mol. weight [g/mol]:	111.12
CAS:	461-87-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	1.529		Crippen Method
mcvol	83.390	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C461870&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

Latest version available from:

<https://www.chemeo.com/cid/92-482-5/C6H6FN.pdf>

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