

1H-Indole, 5-fluoro-

Other names:	Indole, 5-fluoro- 5-Fluoroindole 5-fluoro-1H-indole
Inchi:	InChI=1S/C8H6FN/c9-7-1-2-8-6(5-7)3-4-10-8/h1-5,10H
InchiKey:	ODFFPRGJZRXXNHZ-UHFFFAOYSA-N
Formula:	C8H6FN
SMILES:	Fc1ccc2[nH]ccc2c1
Mol. weight [g/mol]:	135.14
CAS:	399-52-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.83		Crippen Method
logp	1.825		Crippen Method
mcvol	96.410	ml/mol	McGowan Method

Sources

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=C399520&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/40-487-7/1H-Indole-5-fluoro.pdf>

Generated by Cheméo on 2024-04-19 21:30:51.697982272 +0000 UTC m=+15851500.618559584.
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.