

2-(4-Fluorophenyl)indole

Inchi:	InChI=1S/C14H10FN/c15-12-7-5-10(6-8-12)14-9-11-3-1-2-4-13(11)16-14/h1-9,16H
InchiKey:	VLHGDCJIDNVRFM-UHFFFAOYSA-N
Formula:	C14H10FN
SMILES:	Fc1ccc(-c2cc3ccccc3[nH]2)cc1
Mol. weight [g/mol]:	211.23
CAS:	782-17-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.43		Crippen Method
logp	3.492		Crippen Method
mcvol	157.190	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C782172&Units=SI
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

Legend

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

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