

9H-adenine, 2-fluoro-

Inchi:	InChI=1S/C5H4FN5/c6-5-10-3(7)2-4(11-5)9-1-8-2/h1H,(H3,7,8,9,10,11)
InchiKey:	WKMPBTBDYDNUJLF-UHFFFAOYSA-N
Formula:	C5H4FN5
SMILES:	Nc1nc(F)[nH]c2ncnc1-2
Mol. weight [g/mol]:	153.12
CAS:	700-49-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	-0.456		Crippen Method
mcvol	94.060	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=C700492&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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<https://www.chemeo.com/cid/80-842-8/9H-adenine-2-fluoro.pdf>

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