Adenine, 3-(p-fluorobenzyl)-

Inchi:	InChI=1S/C12H10FN5/c13-9-3-1-8(2-4-9)5-18-7-17-11(14)10-12(18)16-6-15-10/h1-4,6-7
InchiKey:	VEXUJFXAZYOOMJ-UHFFFAOYSA-N
Formula:	C12H10FN5
SMILES:	Nc1ncn(Cc2ccc(F)cc2)c2ncnc1-2
Mol. weight [g/mol]:	243.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	1.547		Crippen Method
mcvol	168.930	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=B6009932&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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