

Adenine, 9-benzyl-2-fluoro-

Inchi:	InChI=1S/C12H10FN5/c13-12-16-10(14)9-11(17-12)18(7-15-9)6-8-4-2-1-3-5-8/h1-5,7H,6
InchiKey:	BGMJQNHHBPAADW-UHFFFAOYSA-N
Formula:	C12H10FN5
SMILES:	Nc1nc(F)nc2c1ncn2Cc1ccccc1
Mol. weight [g/mol]:	243.24
CAS:	2357-25-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.10		Crippen Method
logp	1.596		Crippen Method
mcvol	168.930	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=C2357257&Units=SI

Legend

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

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