

# 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,6H2,(H2,14,16,17)

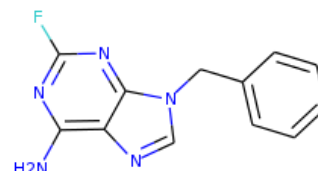
**InChI Key:** BGMJQNHHBPAADW-UHFFFAOYSA-N

**Formula:** C12H10FN5

**SMILES:** Nc1nc(F)nc2c1ncn2Cc1ccccc1

**Molecular Weight:** 243.24

**CAS:** 2357-25-7



## Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	1.60		Crippen Method

## Sources

**NIST Webbook:** [http://webbook.nist.gov/cgi/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,6H2,\(H2,14,16,17\)](http://webbook.nist.gov/cgi/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,6H2,(H2,14,16,17))

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

$\log P_{\text{oct/wat}}$ : Octanol/Water partition coefficient .

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