# Acetamide, n-(5,7-difluoro-1h-benzotriazol-4-yl)-

**Inchi:** InChI=1S/C8H6F2N4O/c1-3(15)11-6-4(9)2-5(10)7-8(6)13-14-12-7/h2H,1H3,(H,11,15)(H,

**InchiKey:** VVWABZRYJMUANY-UHFFFAOYSA-N

**Formula:** C8H6F2N4O

**SMILES:** CC(=O)Nc1c(F)cc(F)c2[nH]nnc12

**Mol. weight [g/mol]:** 212.16

**CAS:** 4140-72-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -2.89 | | Crippen Method |
| logp | 0.713 | | Crippen Method |
| mcvol | 129.690 | ml/mol | McGowan Method |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**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=C4140721&Units=SI

## Legend

**log10ws:** Log10 of Water solubility in mol/l

**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume