

# Allopurinol riboside, tris(trifluoroacetate)

**Inchi:** InChI=1S/C16H9F9N4O8/c17-14(18,19)11(31)34-2-5-6(36-12(32)15(20,21)22)7(37-13(38)39)4-3  
**InchiKey:** CNVLLYZVMIWSKX-UHFFFAOYSA-N  
**Formula:** C16H9F9N4O8  
**SMILES:** O=C(OCC1OC(n2ncc3c(=O)[nH]cnc32)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(F)F)C(F)(F)F  
**Mol. weight [g/mol]:** 556.25

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -3.83   |        | Crippen Method |
| logp          | 0.589   |        | Crippen Method |
| mcvol         | 276.430 | ml/mol | McGowan Method |
| rinpola       | 2303.00 |        | NIST Webbook   |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=U375681&Units=SI>

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**rinpola:** Non-polar retention indices

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