

# D-Allose, pentakis(trifluoroacetate), methyloxime (syn)

**Inchi:** InChI=1S/C17H10F15NO11/c1-39-33-2-4(41-9(35)14(21,22)23)6(43-11(37)16(27,28)29)  
**InchiKey:** IOALWQFXAPVULK-UHFFFAOYSA-N  
**Formula:** C17H10F15NO11  
**SMILES:** CON=CC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)  
**Mol. weight [g/mol]:** 689.24

## Physical Properties

| Property code | Value    | Unit   | Source         |
|---------------|----------|--------|----------------|
| hf            | -4674.73 | kJ/mol | Joback Method  |
| hvap          | 84.65    | kJ/mol | Joback Method  |
| log10ws       | -4.25    |        | Crippen Method |
| logp          | 2.620    |        | Crippen Method |
| mcvol         | 325.690  | ml/mol | McGowan Method |
| pc            | 923.86   | kPa    | Joback Method  |
| rinsol        | 1145.40  |        | NIST Webbook   |
| tb            | 1040.05  | K      | Joback Method  |
| tc            | 1307.10  | K      | Joback Method  |

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U380246&Units=SI>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l

|                |                                     |
|----------------|-------------------------------------|
| <b>logp:</b>   | Octanol/Water partition coefficient |
| <b>mcvol:</b>  | McGowan's characteristic volume     |
| <b>pc:</b>     | Critical Pressure                   |
| <b>rinpol:</b> | Non-polar retention indices         |
| <b>tb:</b>     | Normal Boiling Point Temperature    |
| <b>tc:</b>     | Critical Temperature                |

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