

# 2-Deoxy-D-ribose, tris(trifluoroacetate), methyloxime (isomer 2)

**InChI:** InChI=1S/C12H10F9NO7/c1-26-22-3-2-5(28-8(24)11(16,17)18)6(29-9(25)12(19,20)21)4-27-7(23)10(13,14)15/h3,5-6H,2,4H2,1H3

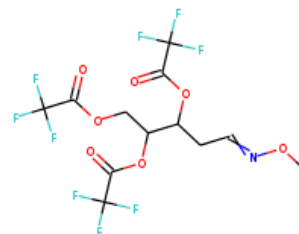
**InChI Key:** VKXDKGHDCPATCL-UHFFFAOYSA-N

**Formula:** C12H10F9NO7

**SMILES:**

CON=CCC(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F

**Molecular Weight:** 451.20



## Physical Properties

| Property                        | Value    | Unit   | Source         |
|---------------------------------|----------|--------|----------------|
| $\Delta_f H^\circ_{\text{gas}}$ | -2877.21 | kJ/mol | Joback Method  |
| $\Delta_{\text{vap}} H^\circ$   | 63.48    | kJ/mol | Joback Method  |
| $\log P_{\text{oct/wat}}$       | 2.06     |        | Crippen Method |
| $P_c$                           | 1386.08  | kPa    | Joback Method  |
| $T_{\text{boil}}$               | 784.79   | K      | Joback Method  |
| $T_c$                           | 964.80   | K      | Joback Method  |

## Sources

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**NIST Webbook:** [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H10F9NO7/c1-26-22-3-2-5\(28-8\(24\)11\(16,17\)18\)6\(29-9\(25\)12\(19,20\)21\)4-27-7\(23\)10\(13,14\)15/h3,5-6H,2,4H2,1H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H10F9NO7/c1-26-22-3-2-5(28-8(24)11(16,17)18)6(29-9(25)12(19,20)21)4-27-7(23)10(13,14)15/h3,5-6H,2,4H2,1H3)

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

## Legend

$\Delta_f H^\circ_{\text{gas}}$ : Enthalpy of formation at standard conditions (kJ/mol).

$\Delta_{\text{vap}} H^\circ$ : Enthalpy of vaporization at standard conditions (kJ/mol).

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

$P_c$ : Critical Pressure (kPa).

$T_{\text{boil}}$ : Normal Boiling Point Temperature (K).  
 $T_{\text{c}}$ : Critical Temperature (K).

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