# L-(+)-Threose, tris(trifluoroacetate), methyloxime (anti)

**Inchi:** InChI=1S/C11H8F9NO7/c1-25-21-2-4(27-7(23)10(15,16)17)5(28-8(24)11(18,19)20)3-26-

**InchiKey:** LXLUTTKJBAJCOL-UHFFFAOYSA-N

**Formula:** C11H8F9NO7

**SMILES:** CON=CC(OC(=O)C(F)(F)F)C(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F

**Mol. weight [g/mol]:** 437.17

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -2856.57 | kJ/mol | Joback Method |
| hvap | 61.26 | kJ/mol | Joback Method |
| log10ws | -2.47 | | Crippen Method |
| logp | 1.672 | | Crippen Method |
| mcvol | 215.650 | ml/mol | McGowan Method |
| pc | 1490.74 | kPa | Joback Method |
| rinpol | 1031.30 | | NIST Webbook |
| rinpol | 1031.30 | | NIST Webbook |
| tb | 761.91 | K | Joback Method |
| tc | 939.63 | K | Joback Method |

## Sources

**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=U380241&Units=SI

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

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

## Legend

**hf:** Enthalpy of formation at standard conditions

**hvap:** Enthalpy of vaporization at standard conditions

| | |
|---|---|
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |

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