# L-Sorbopyranose, pentakis(trifluoroacetate) (isomer 1)

**Inchi:** InChI=1S/C16H7F15O11/c17-12(18,19)6(32)37-2-11(42-10(36)16(29,30)31)5(41-9(35)15
**InchiKey:** TVXVQZUZYLRUBY-UHFFFAOYSA-N
**Formula:** C16H7F15O11
**SMILES:** O=C(OCC1(OC(=O)C(F)(F)F)OCC(OC(=O)C(F)(F)F)C(OC(=O)C(F)(F)F)C1OC(=O)C(F)(
**Mol. weight [g/mol]:** 660.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -4084.00 | kJ/mol | Joback Method |
| hf | -4706.43 | kJ/mol | Joback Method |
| hfus | 56.99 | kJ/mol | Joback Method |
| hvap | 81.12 | kJ/mol | Joback Method |
| log10ws | -4.07 | | Crippen Method |
| logp | 2.346 | | Crippen Method |
| mcvol | 295.060 | ml/mol | McGowan Method |
| pc | 1139.80 | kPa | Joback Method |
| rinpol | 1132.50 | | NIST Webbook |
| rinpol | 1132.50 | | NIST Webbook |
| tb | 952.56 | K | Joback Method |
| tc | 1173.44 | K | Joback Method |
| tf | 696.96 | K | Joback Method |
| vc | 1.216 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1013.67 | J/mol×K | 952.56 | Joback Method |
| cpg | 1024.63 | J/mol×K | 989.37 | Joback Method |
| cpg | 1035.04 | J/mol×K | 1026.19 | Joback Method |
| cpg | 1045.07 | J/mol×K | 1063.00 | Joback Method |
| cpg | 1054.87 | J/mol×K | 1099.82 | Joback Method |
| cpg | 1064.59 | J/mol×K | 1136.63 | Joback Method |
| cpg | 1074.39 | J/mol×K | 1173.44 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **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=U380292&Units=SI |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion 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 |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |