# (2R,3R)-(-)-2-Benzyloxy-1,3,4-butanetriol, tris(trifluoroacetate)

**Inchi:** InChI=1S/C17H13F9O7/c18-15(19,20)12(27)31-7-10(30-6-9-4-2-1-3-5-9)11(33-14(29)17
**InchiKey:** QVSPLHGYEGENNA-UHFFFAOYSA-N
**Formula:** C17H13F9O7
**SMILES:** O=C(OCC(OCc1ccccc1)C(COC(=O)C(F)(F)F)OC(=O)C(F)(F)F)C(F)(F)F
**Mol. weight [g/mol]:** 500.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -2351.74 | kJ/mol | Joback Method |
| hf | -2826.10 | kJ/mol | Joback Method |
| hfus | 41.81 | kJ/mol | Joback Method |
| hvap | 73.57 | kJ/mol | Joback Method |
| log10ws | -4.42 | | Crippen Method |
| logp | 3.257 | | Crippen Method |
| mcvol | 270.750 | ml/mol | McGowan Method |
| pc | 1341.76 | kPa | Joback Method |
| rinpol | 1496.10 | | NIST Webbook |
| tb | 849.19 | K | Joback Method |
| tc | 1041.35 | K | Joback Method |
| tf | 529.05 | K | Joback Method |
| vc | 1.087 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 847.81 | J/mol×K | 849.19 | Joback Method |
| cpg | 858.10 | J/mol×K | 881.22 | Joback Method |
| cpg | 867.40 | J/mol×K | 913.24 | Joback Method |
| cpg | 875.76 | J/mol×K | 945.27 | Joback Method |
| cpg | 883.24 | J/mol×K | 977.29 | Joback Method |
| cpg | 889.87 | J/mol×K | 1009.32 | Joback Method |
| cpg | 895.70 | J/mol×K | 1041.35 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U380215&Units=SI |
| **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 |

# 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 |