# 2,3,4-Trifluorobenzoic acid, 4-benzyloxyphenyl ester

**Inchi:** InChI=1S/C20H13F3O3/c21-17-11-10-16(18(22)19(17)23)20(24)26-15-8-6-14(7-9-15)25-
**InchiKey:** LSPRJYJEPMKXBQ-UHFFFAOYSA-N
**Formula:** C20H13F3O3
**SMILES:** O=C(Oc1ccc(OCc2ccccc2)cc1)c1ccc(F)c(F)c1F
**Mol. weight [g/mol]:** 358.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -507.12 | kJ/mol | Joback Method |
| hf | -757.77 | kJ/mol | Joback Method |
| hfus | 41.34 | kJ/mol | Joback Method |
| hvap | 78.70 | kJ/mol | Joback Method |
| log10ws | -6.78 | | Crippen Method |
| logp | 4.902 | | Crippen Method |
| mcvol | 240.000 | ml/mol | McGowan Method |
| pc | 1872.41 | kPa | Joback Method |
| rinpol | 2548.00 | | NIST Webbook |
| rinpol | 2548.00 | | NIST Webbook |
| tb | 853.48 | K | Joback Method |
| tc | 1082.48 | K | Joback Method |
| tf | 540.66 | K | Joback Method |
| vc | 0.927 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 689.75 | J/mol×K | 853.48 | Joback Method |
| cpg | 702.13 | J/mol×K | 891.65 | Joback Method |
| cpg | 713.27 | J/mol×K | 929.81 | Joback Method |
| cpg | 723.21 | J/mol×K | 967.98 | Joback Method |
| cpg | 731.97 | J/mol×K | 1006.15 | Joback Method |
| cpg | 739.60 | J/mol×K | 1044.31 | Joback Method |
| cpg | 746.12 | J/mol×K | 1082.48 | Joback Method |

# Sources

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|---|---|
| **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=U308038&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |