# 3-Methoxy-2,4,5-trifluorobenzoic acid, 4-biphenyl ester

**Inchi:** InChI=1S/C20H13F3O3/c1-25-19-17(22)15(11-16(21)18(19)23)20(24)26-14-9-7-13(8-10-

**InchiKey:** RWANLUGHJXIBLA-UHFFFAOYSA-N

**Formula:** C20H13F3O3

**SMILES:** COc1c(F)c(F)cc(C(=O)Oc2ccc(-c3ccccc3)cc2)c1F

**Mol. weight [g/mol]:** 358.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -516.75 | kJ/mol | Joback Method |
| hf | -769.24 | kJ/mol | Joback Method |
| hfus | 40.95 | kJ/mol | Joback Method |
| hvap | 79.37 | kJ/mol | Joback Method |
| log10ws | -7.28 | | Crippen Method |
| logp | 4.999 | | Crippen Method |
| mcvol | 240.000 | ml/mol | McGowan Method |
| pc | 1848.33 | kPa | Joback Method |
| rinpol | 2654.00 | | NIST Webbook |
| tb | 858.46 | K | Joback Method |
| tc | 1088.20 | K | Joback Method |
| tf | 553.18 | K | Joback Method |
| vc | 0.927 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 688.32 | J/mol×K | 858.46 | Joback Method |
| cpg | 700.61 | J/mol×K | 896.75 | Joback Method |
| cpg | 711.64 | J/mol×K | 935.04 | Joback Method |
| cpg | 721.46 | J/mol×K | 973.33 | Joback Method |
| cpg | 730.09 | J/mol×K | 1011.62 | Joback Method |
| cpg | 737.56 | J/mol×K | 1049.91 | Joback Method |
| cpg | 743.88 | J/mol×K | 1088.20 | 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=U360577&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |