# 2-Trifluoromethylbenzoic acid, 2-bromo-4-fluorophenyl ester

**Inchi:** InChI=1S/C14H7BrF4O2/c15-11-7-8(16)5-6-12(11)21-13(20)9-3-1-2-4-10(9)14(17,18)19/

**InchiKey:** TZOAFPPYRMIKQT-UHFFFAOYSA-N

**Formula:** C14H7BrF4O2

**SMILES:** O=C(Oc1ccc(F)cc1Br)c1ccccc1C(F)(F)F

**Mol. weight [g/mol]:** 363.10

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -733.07 | kJ/mol | Joback Method |
| hf | -905.30 | kJ/mol | Joback Method |
| hfus | 31.91 | kJ/mol | Joback Method |
| hvap | 64.32 | kJ/mol | Joback Method |
| log10ws | -6.16 | | Crippen Method |
| logp | 4.826 | | Crippen Method |
| mcvol | 192.620 | ml/mol | McGowan Method |
| pc | 2522.65 | kPa | Joback Method |
| rinpol | 1874.00 | | NIST Webbook |
| rinpol | 1874.00 | | NIST Webbook |
| tb | 724.32 | K | Joback Method |
| tc | 950.72 | K | Joback Method |
| tf | 474.68 | K | Joback Method |
| vc | 0.750 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 481.93 | J/mol×K | 724.32 | Joback Method |
| cpg | 492.73 | J/mol×K | 762.05 | Joback Method |
| cpg | 502.59 | J/mol×K | 799.79 | Joback Method |
| cpg | 511.57 | J/mol×K | 837.52 | Joback Method |
| cpg | 519.74 | J/mol×K | 875.25 | Joback Method |
| cpg | 527.16 | J/mol×K | 912.99 | Joback Method |
| cpg | 533.90 | J/mol×K | 950.72 | Joback Method |

# Sources

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|---|---|
| **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=U299012&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |