# MPMC, TFA

**Inchi:** InChI=1S/C12H12F3NO3/c1-7-4-5-9(6-8(7)2)19-11(18)16(3)10(17)12(13,14)15/h4-6H,1-
**InchiKey:** SAIIMSPDMSJCQF-UHFFFAOYSA-N
**Formula:** C12H12F3NO3
**SMILES:** Cc1ccc(OC(=O)N(C)C(=O)C(F)(F)F)cc1C
**Mol. weight [g/mol]:** 275.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -690.34 | kJ/mol | Joback Method |
| hf | -964.35 | kJ/mol | Joback Method |
| hfus | 29.33 | kJ/mol | Joback Method |
| hvap | 60.10 | kJ/mol | Joback Method |
| log10ws | -3.56 | | Crippen Method |
| logp | 2.823 | | Crippen Method |
| mcvol | 180.480 | ml/mol | McGowan Method |
| pc | 2315.84 | kPa | Joback Method |
| rinpol | 1526.00 | | NIST Webbook |
| rinpol | 1526.00 | | NIST Webbook |
| rinpol | 1519.00 | | NIST Webbook |
| tb | 647.78 | K | Joback Method |
| tc | 844.48 | K | Joback Method |
| tf | 435.21 | K | Joback Method |
| vc | 0.691 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 475.39 | J/mol×K | 647.78 | Joback Method |
| cpg | 487.83 | J/mol×K | 680.56 | Joback Method |
| cpg | 499.44 | J/mol×K | 713.35 | Joback Method |
| cpg | 510.27 | J/mol×K | 746.13 | Joback Method |
| cpg | 520.34 | J/mol×K | 778.91 | Joback Method |
| cpg | 529.68 | J/mol×K | 811.70 | Joback Method |
| cpg | 538.34 | J/mol×K | 844.48 | 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=R522140&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 |

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