# Pyridine-3,5-dicarboxylic acid, 1,4-dihydro-2,6-dimethyl-4-(o-trifluoromethylphen diethyl ester

**InChI:** InChI=1S/C20H22F3NO4/c1-5-27-18(25)15-11(3)24-12(4)16(19(26)28-6-2)17(15)13-9-7-
**InChIKey:** ACZJZGLXRPZSLI-UHFFFAOYSA-N
**Formula:** C20H22F3NO4
**SMILES:** CCOC(=O)C1=C(C)NC(C)=C(C(=O)OCC)C1c1ccccc1C(F)(F)F
**Mol. weight [g/mol]:** 397.39
**CAS:** 23191-75-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -695.57 | kJ/mol | Joback Method |
| hf | -1155.94 | kJ/mol | Joback Method |
| hfus | 50.92 | kJ/mol | Joback Method |
| hvap | 88.04 | kJ/mol | Joback Method |
| log10ws | -5.45 | | Crippen Method |
| logp | 4.066 | | Crippen Method |
| mcvol | 279.610 | ml/mol | McGowan Method |
| pc | 1474.75 | kPa | Joback Method |
| tb | 922.16 | K | Joback Method |
| tc | 1141.57 | K | Joback Method |
| tf | 666.62 | K | Joback Method |
| vc | 1.081 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 883.13 | J/mol×K | 922.16 | Joback Method |
| cpg | 895.96 | J/mol×K | 958.73 | Joback Method |
| cpg | 907.45 | J/mol×K | 995.30 | Joback Method |
| cpg | 917.61 | J/mol×K | 1031.86 | Joback Method |
| cpg | 926.47 | J/mol×K | 1068.43 | Joback Method |
| cpg | 934.04 | J/mol×K | 1105.00 | Joback Method |
| cpg | 940.35 | J/mol×K | 1141.57 | 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=C23191755&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |