# 2-(Ethyl(m-tolyl)amino)ethyl 2,3,4,5,6-pentafluorobenzoate

**Inchi:** InChI=1S/C18H16F5NO2/c1-3-24(11-6-4-5-10(2)9-11)7-8-26-18(25)12-13(19)15(21)17(2

**InchiKey:** MBIZDDGNLXPDRM-UHFFFAOYSA-N

**Formula:** C18H16F5NO2

**SMILES:** CCN(CCOC(=O)c1c(F)c(F)c(F)c(F)c1F)c1cccc(C)c1

**Mol. weight [g/mol]:** 373.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -829.47 | kJ/mol | Joback Method |
| hf | -1168.43 | kJ/mol | Joback Method |
| hfus | 49.33 | kJ/mol | Joback Method |
| hvap | 71.30 | kJ/mol | Joback Method |
| log10ws | -5.82 | | Crippen Method |
| logp | 4.374 | | Crippen Method |
| mcvol | 243.230 | ml/mol | McGowan Method |
| pc | 1531.86 | kPa | Joback Method |
| rinpol | 2069.00 | | NIST Webbook |
| tb | 779.56 | K | Joback Method |
| tc | 972.47 | K | Joback Method |
| tf | 528.16 | K | Joback Method |
| vc | 0.960 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 700.11 | J/mol×K | 779.56 | Joback Method |
| cpg | 713.28 | J/mol×K | 811.71 | Joback Method |
| cpg | 725.58 | J/mol×K | 843.86 | Joback Method |
| cpg | 737.02 | J/mol×K | 876.02 | Joback Method |
| cpg | 747.64 | J/mol×K | 908.17 | Joback Method |
| cpg | 757.44 | J/mol×K | 940.32 | Joback Method |
| cpg | 766.46 | J/mol×K | 972.47 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373602&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# 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 |