# N-(2-Ethoxyphenyl)-N-2,2,2-trifluoroacetyl-2,2,2-tr

**Inchi:** InChI=1S/C12H9F6NO3/c1-2-22-8-6-4-3-5-7(8)19(9(20)11(13,14)15)10(21)12(16,17)18/h
**InchiKey:** WGJJMKHKRFBNIM-UHFFFAOYSA-N
**Formula:** C12H9F6NO3
**SMILES:** CCOc1ccccc1N(C(=O)C(F)(F)F)C(=O)C(F)(F)F
**Mol. weight [g/mol]:** 329.20

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1262.30 | kJ/mol | Joback Method |
| hf | -1549.96 | kJ/mol | Joback Method |
| hfus | 31.55 | kJ/mol | Joback Method |
| hvap | 55.70 | kJ/mol | Joback Method |
| log10ws | -3.63 | | Crippen Method |
| logp | 3.070 | | Crippen Method |
| mcvol | 185.790 | ml/mol | McGowan Method |
| pc | 2106.13 | kPa | Joback Method |
| rinpol | 1229.00 | | NIST Webbook |
| rinpol | 1229.00 | | NIST Webbook |
| tb | 637.38 | K | Joback Method |
| tc | 819.84 | K | Joback Method |
| tf | 426.88 | K | Joback Method |
| vc | 0.734 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 503.81 | J/mol×K | 637.38 | Joback Method |
| cpg | 515.32 | J/mol×K | 667.79 | Joback Method |
| cpg | 525.99 | J/mol×K | 698.20 | Joback Method |
| cpg | 535.89 | J/mol×K | 728.61 | Joback Method |
| cpg | 545.04 | J/mol×K | 759.02 | Joback Method |
| cpg | 553.49 | J/mol×K | 789.43 | Joback Method |
| cpg | 561.30 | J/mol×K | 819.84 | 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=U373207&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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