# 4-Hexylphenyl trifluoroacetate

**Inchi:** InChI=1S/C14H17F3O2/c1-2-3-4-5-6-11-7-9-12(10-8-11)19-13(18)14(15,16)17/h7-10H,2
**InchiKey:** YQQNYIXNCOSQFQ-UHFFFAOYSA-N
**Formula:** C14H17F3O2
**SMILES:** CCCCCCc1ccc(OC(=O)C(F)(F)F)cc1
**Mol. weight [g/mol]:** 274.28

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -645.73 | kJ/mol | Joback Method |
| hf | -949.11 | kJ/mol | Joback Method |
| hfus | 30.28 | kJ/mol | Joback Method |
| hvap | 55.11 | kJ/mol | Joback Method |
| log10ws | -4.92 | | Crippen Method |
| logp | 4.277 | | Crippen Method |
| mcvol | 197.110 | ml/mol | McGowan Method |
| pc | 1864.33 | kPa | Joback Method |
| rinpol | 1435.00 | | NIST Webbook |
| rinpol | 1435.00 | | NIST Webbook |
| tb | 622.25 | K | Joback Method |
| tc | 808.73 | K | Joback Method |
| tf | 362.83 | K | Joback Method |
| vc | 0.778 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 521.05 | J/mol×K | 622.25 | Joback Method |
| cpg | 535.79 | J/mol×K | 653.33 | Joback Method |
| cpg | 549.69 | J/mol×K | 684.41 | Joback Method |
| cpg | 562.77 | J/mol×K | 715.49 | Joback Method |
| cpg | 575.06 | J/mol×K | 746.57 | Joback Method |
| cpg | 586.61 | J/mol×K | 777.65 | Joback Method |
| cpg | 597.44 | J/mol×K | 808.73 | 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=U373440&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 |