# (.+/-.)-Lavandulol, chlorodifluoroacetate

**Inchi:** InChI=1S/C12H17ClF2O2/c1-8(2)5-6-10(9(3)4)7-17-11(16)12(13,14)15/h5,10H,3,6-7H2,1
**InchiKey:** AYASINNVPARBCO-UHFFFAOYSA-N
**Formula:** C12H17ClF2O2
**SMILES:** C=C(C)C(CC=C(C)C)COC(=O)C(F)(F)Cl
**Mol. weight [g/mol]:** 266.71

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -433.95 | kJ/mol | Joback Method |
| hf | -734.73 | kJ/mol | Joback Method |
| hfus | 25.34 | kJ/mol | Joback Method |
| hvap | 51.98 | kJ/mol | Joback Method |
| log10ws | -4.14 | | Crippen Method |
| logp | 3.910 | | Crippen Method |
| mcvol | 194.560 | ml/mol | McGowan Method |
| pc | 1857.91 | kPa | Joback Method |
| tb | 583.15 | K | Joback Method |
| tc | 770.17 | K | Joback Method |
| tf | 280.92 | K | Joback Method |
| vc | 0.762 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 475.39 | J/mol×K | 583.15 | Joback Method |
| cpg | 489.58 | J/mol×K | 614.32 | Joback Method |
| cpg | 502.95 | J/mol×K | 645.49 | Joback Method |
| cpg | 515.55 | J/mol×K | 676.66 | Joback Method |
| cpg | 527.42 | J/mol×K | 707.83 | Joback Method |
| cpg | 538.60 | J/mol×K | 739.00 | Joback Method |
| cpg | 549.12 | J/mol×K | 770.17 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U376229&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |