# (Phenylthio)acetic acid, (4-chlorophenyl)methyl ester

**Inchi:** InChI=1S/C15H13ClO2S/c16-13-8-6-12(7-9-13)10-18-15(17)11-19-14-4-2-1-3-5-14/h1-9
**InchiKey:** ZHIZABUTNCVGJX-UHFFFAOYSA-N
**Formula:** C15H13ClO2S
**SMILES:** O=C(CSc1ccccc1)OCc1ccc(Cl)cc1
**Mol. weight [g/mol]:** 292.78

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 77.88 | kJ/mol | Joback Method |
| hf | -110.01 | kJ/mol | Joback Method |
| hfus | 33.41 | kJ/mol | Joback Method |
| hvap | 74.56 | kJ/mol | Joback Method |
| log10ws | -4.71 | | Crippen Method |
| logp | 4.175 | | Crippen Method |
| mcvol | 210.720 | ml/mol | McGowan Method |
| pc | 2537.93 | kPa | Joback Method |
| rinpol | 2242.00 | | NIST Webbook |
| tb | 783.44 | K | Joback Method |
| tc | 1039.18 | K | Joback Method |
| tf | 460.65 | K | Joback Method |
| vc | 0.786 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 541.44 | J/mol×K | 783.44 | Joback Method |
| cpg | 554.66 | J/mol×K | 826.06 | Joback Method |
| cpg | 566.56 | J/mol×K | 868.69 | Joback Method |
| cpg | 577.19 | J/mol×K | 911.31 | Joback Method |
| cpg | 586.61 | J/mol×K | 953.93 | Joback Method |
| cpg | 594.86 | J/mol×K | 996.55 | Joback Method |
| cpg | 602.00 | J/mol×K | 1039.18 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U308340&Units=SI |

# 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 |