# Phthalic acid, dodecyl 4-methylthiophenyl ester

**Inchi:** InChI=1S/C27H36O4S/c1-3-4-5-6-7-8-9-10-11-14-21-30-26(28)24-15-12-13-16-25(24)27

**InchiKey:** VILBCMSDDKNXON-UHFFFAOYSA-N

**Formula:** C27H36O4S

**SMILES:** CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1ccc(SC)cc1

**Mol. weight [g/mol]:** 456.64

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -52.70 | kJ/mol | Joback Method |
| hf | -598.22 | kJ/mol | Joback Method |
| hfus | 62.69 | kJ/mol | Joback Method |
| hvap | 106.70 | kJ/mol | Joback Method |
| log10ws | -9.15 | | Crippen Method |
| logp | 7.705 | | Crippen Method |
| mcvol | 375.000 | ml/mol | McGowan Method |
| pc | 1061.71 | kPa | Joback Method |
| rinpol | 1487.00 | | NIST Webbook |
| rinpol | 1487.00 | | NIST Webbook |
| tb | 1101.84 | K | Joback Method |
| tc | 1348.97 | K | Joback Method |
| tf | 650.65 | K | Joback Method |
| vc | 1.433 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1247.91 | J/mol×K | 1101.84 | Joback Method |
| cpg | 1259.58 | J/mol×K | 1143.03 | Joback Method |
| cpg | 1269.43 | J/mol×K | 1184.22 | Joback Method |
| cpg | 1277.51 | J/mol×K | 1225.40 | Joback Method |
| cpg | 1283.90 | J/mol×K | 1266.59 | Joback Method |
| cpg | 1288.66 | J/mol×K | 1307.78 | Joback Method |
| cpg | 1291.84 | J/mol×K | 1348.97 | 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=U415621&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 |