# Phthalic acid, 4-chloro-2-methoxybenzyl dodecyl ester

**Inchi:** InChI=1S/C28H37ClO5/c1-3-4-5-6-7-8-9-10-11-14-19-33-27(30)24-15-12-13-16-25(24)28

**InchiKey:** WXROEQMAFPMRPJ-UHFFFAOYSA-N

**Formula:** C28H37ClO5

**SMILES:** CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(Cl)cc1OC

**Mol. weight [g/mol]:** 489.04

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -203.96 | kJ/mol | Joback Method |
| hf | -820.16 | kJ/mol | Joback Method |
| hfus | 66.15 | kJ/mol | Joback Method |
| hvap | 109.57 | kJ/mol | Joback Method |
| log10ws | -9.48 | | Crippen Method |
| logp | 7.783 | | Crippen Method |
| mcvol | 390.850 | ml/mol | McGowan Method |
| pc | 946.16 | kPa | Joback Method |
| rinpol | 3473.00 | | NIST Webbook |
| rinpol | 3473.00 | | NIST Webbook |
| tb | 1120.77 | K | Joback Method |
| tc | 1374.61 | K | Joback Method |
| tf | 692.19 | K | Joback Method |
| vc | 1.502 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1303.81 | J/mol×K | 1120.77 | Joback Method |
| cpg | 1340.66 | J/mol×K | 1332.30 | Joback Method |
| cpg | 1337.18 | J/mol×K | 1289.99 | Joback Method |
| cpg | 1331.82 | J/mol×K | 1247.69 | Joback Method |
| cpg | 1324.50 | J/mol×K | 1205.38 | Joback Method |
| cpg | 1315.19 | J/mol×K | 1163.08 | Joback Method |
| cpg | 1342.31 | J/mol×K | 1374.61 | Joback Method |
| dvisc | 0.0000113 | Pa×s | 1120.77 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000143 | Pa×s | 1049.34 | Joback Method |
| dvisc | 0.0000188 | Pa×s | 977.91 | Joback Method |
| dvisc | 0.0000257 | Pa×s | 906.48 | Joback Method |
| dvisc | 0.0000371 | Pa×s | 835.05 | Joback Method |
| dvisc | 0.0000573 | Pa×s | 763.62 | Joback Method |
| dvisc | 0.0000969 | Pa×s | 692.19 | Joback Method |

# Sources

| | |
|---|---|
| **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=U382846&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |