# Phthalic acid, decyl 4-methylhept-3-yl ester

**Inchi:** InChI=1S/C26H42O4/c1-5-8-9-10-11-12-13-16-20-29-25(27)22-18-14-15-19-23(22)26(28
**InchiKey:** ZQBKBFFQXKFTBE-UHFFFAOYSA-N
**Formula:** C26H42O4
**SMILES:** CCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(CC)C(C)CCC
**Mol. weight [g/mol]:** 418.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -201.90 | kJ/mol | Joback Method |
| hf | -855.07 | kJ/mol | Joback Method |
| hfus | 55.28 | kJ/mol | Joback Method |
| hvap | 93.94 | kJ/mol | Joback Method |
| log10ws | -8.52 | | Crippen Method |
| logp | 7.356 | | Crippen Method |
| mcvol | 368.320 | ml/mol | McGowan Method |
| pc | 923.86 | kPa | Joback Method |
| rinpol | 2793.00 | | NIST Webbook |
| rinpol | 2793.00 | | NIST Webbook |
| tb | 977.64 | K | Joback Method |
| tc | 1196.94 | K | Joback Method |
| tf | 536.04 | K | Joback Method |
| vc | 1.419 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1244.40 | J/mol×K | 977.64 | Joback Method |
| cpg | 1261.82 | J/mol×K | 1014.19 | Joback Method |
| cpg | 1277.68 | J/mol×K | 1050.74 | Joback Method |
| cpg | 1292.02 | J/mol×K | 1087.29 | Joback Method |
| cpg | 1304.91 | J/mol×K | 1123.84 | Joback Method |
| cpg | 1316.39 | J/mol×K | 1160.39 | Joback Method |
| cpg | 1326.50 | J/mol×K | 1196.94 | Joback Method |
| dvisc | 0.0003771 | Pa×s | 536.04 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001694 | Pa×s | 609.64 | Joback Method |
| dvisc | 0.0000904 | Pa×s | 683.24 | Joback Method |
| dvisc | 0.0000545 | Pa×s | 756.84 | Joback Method |
| dvisc | 0.0000360 | Pa×s | 830.44 | Joback Method |
| dvisc | 0.0000254 | Pa×s | 904.04 | Joback Method |
| dvisc | 0.0000189 | Pa×s | 977.64 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U377945&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

| | |
|---|---|
| **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 |