# 2,4-Ditert-butyl-6-chlorophenyl phenylacetate

**Inchi:** InChI=1S/C22H27ClO2/c1-21(2,3)16-13-17(22(4,5)6)20(18(23)14-16)25-19(24)12-15-10-
**InchiKey:** NSDNNCDBSGFZIE-UHFFFAOYSA-N
**Formula:** C22H27ClO2
**SMILES:** CC(C)(C)c1cc(Cl)c(OC(=O)Cc2ccccc2)c(C(C)(C)C)c1
**Mol. weight [g/mol]:** 358.90
**CAS:** 116296-26-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 90.12 | kJ/mol | Joback Method |
| hf | -336.80 | kJ/mol | Joback Method |
| hfus | 31.81 | kJ/mol | Joback Method |
| hvap | 82.05 | kJ/mol | Joback Method |
| log10ws | -6.71 | | Crippen Method |
| logp | 6.083 | | Crippen Method |
| mcvol | 293.000 | ml/mol | McGowan Method |
| pc | 1406.95 | kPa | Joback Method |
| tb | 878.32 | K | Joback Method |
| tc | 1115.43 | K | Joback Method |
| tf | 535.02 | K | Joback Method |
| vc | 1.103 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 880.77 | J/mol×K | 878.32 | Joback Method |
| cpg | 896.99 | J/mol×K | 917.84 | Joback Method |
| cpg | 911.98 | J/mol×K | 957.36 | Joback Method |
| cpg | 925.83 | J/mol×K | 996.87 | Joback Method |
| cpg | 938.67 | J/mol×K | 1036.39 | Joback Method |
| cpg | 950.62 | J/mol×K | 1075.91 | Joback Method |
| cpg | 961.79 | J/mol×K | 1115.43 | Joback Method |
| dvisc | 0.0003617 | Pa×s | 535.02 | Joback Method |
| dvisc | 0.0001988 | Pa×s | 592.24 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001214 | Pa×s | 649.45 | Joback Method |
| dvisc | 0.0000803 | Pa×s | 706.67 | Joback Method |
| dvisc | 0.0000565 | Pa×s | 763.89 | Joback Method |
| dvisc | 0.0000417 | Pa×s | 821.10 | Joback Method |
| dvisc | 0.0000321 | Pa×s | 878.32 | Joback Method |

# Sources

| | |
|---|---|
| **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=C116296265&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |