# Isophthalic acid, 2,6-dichlorophenyl pentyl ester

**Inchi:** InChI=1S/C19H18Cl2O4/c1-2-3-4-11-24-18(22)13-7-5-8-14(12-13)19(23)25-17-15(20)9-6

**InchiKey:** BHGCTCFKEWKOKR-UHFFFAOYSA-N

**Formula:** C19H18Cl2O4

**SMILES:** CCCCCOC(=O)c1cccc(C(=O)Oc2c(Cl)cccc2Cl)c1

**Mol. weight [g/mol]:** 381.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -186.67 | kJ/mol | Joback Method |
| hf | -517.92 | kJ/mol | Joback Method |
| hfus | 45.85 | kJ/mol | Joback Method |
| hvap | 91.51 | kJ/mol | Joback Method |
| log10ws | -6.85 | | Crippen Method |
| logp | 5.560 | | Crippen Method |
| mcvol | 270.410 | ml/mol | McGowan Method |
| pc | 1726.03 | kPa | Joback Method |
| rinpol | 2843.00 | | NIST Webbook |
| rinpol | 2843.00 | | NIST Webbook |
| tb | 929.86 | K | Joback Method |
| tc | 1163.73 | K | Joback Method |
| tf | 598.45 | K | Joback Method |
| vc | 1.030 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 765.86 | J/mol×K | 929.86 | Joback Method |
| cpg | 776.98 | J/mol×K | 968.84 | Joback Method |
| cpg | 786.84 | J/mol×K | 1007.82 | Joback Method |
| cpg | 795.46 | J/mol×K | 1046.79 | Joback Method |
| cpg | 802.88 | J/mol×K | 1085.77 | Joback Method |
| cpg | 809.13 | J/mol×K | 1124.75 | Joback Method |
| cpg | 814.22 | J/mol×K | 1163.73 | Joback Method |
| dvisc | 0.0003155 | Pa×s | 598.45 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002039 | Pa×s | 653.69 | Joback Method |
| dvisc | 0.0001411 | Pa×s | 708.92 | Joback Method |
| dvisc | 0.0001029 | Pa×s | 764.15 | Joback Method |
| dvisc | 0.0000784 | Pa×s | 819.39 | Joback Method |
| dvisc | 0.0000617 | Pa×s | 874.62 | Joback Method |
| dvisc | 0.0000500 | Pa×s | 929.86 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U344622&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |

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