# Succinic acid, 2-isopropoxyphenyl 2,4-dichloro-6-formylphenyl ester

**Inchi:** InChI=1S/C20H18Cl2O6/c1-12(2)26-16-5-3-4-6-17(16)27-18(24)7-8-19(25)28-20-13(11-2

**InchiKey:** PXITZQGGEPDSKB-UHFFFAOYSA-N

**Formula:** C20H18Cl2O6

**SMILES:** CC(C)Oc1ccccc1OC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1C=O

**Mol. weight [g/mol]:** 425.26

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -394.84 | kJ/mol | Joback Method |
| hf | -773.11 | kJ/mol | Joback Method |
| hfus | 48.00 | kJ/mol | Joback Method |
| hvap | 103.14 | kJ/mol | Joback Method |
| log10ws | -6.43 | | Crippen Method |
| logp | 4.884 | | Crippen Method |
| mcvol | 291.940 | ml/mol | McGowan Method |
| pc | 1661.90 | kPa | Joback Method |
| rinpol | 3037.00 | | NIST Webbook |
| rinpol | 3037.00 | | NIST Webbook |
| tb | 1028.36 | K | Joback Method |
| tc | 1268.89 | K | Joback Method |
| tf | 671.47 | K | Joback Method |
| vc | 1.115 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 849.74 | J/mol×K | 1028.36 | Joback Method |
| cpg | 857.44 | J/mol×K | 1068.45 | Joback Method |
| cpg | 863.57 | J/mol×K | 1108.54 | Joback Method |
| cpg | 868.14 | J/mol×K | 1148.63 | Joback Method |
| cpg | 871.14 | J/mol×K | 1188.72 | Joback Method |
| cpg | 872.57 | J/mol×K | 1228.80 | Joback Method |
| cpg | 872.46 | J/mol×K | 1268.89 | Joback Method |
| dvisc | 0.0001947 | Pa×s | 671.47 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001276 | Pa×s | 730.95 | Joback Method |
| dvisc | 0.0000891 | Pa×s | 790.43 | Joback Method |
| dvisc | 0.0000654 | Pa×s | 849.91 | Joback Method |
| dvisc | 0.0000500 | Pa×s | 909.40 | Joback Method |
| dvisc | 0.0000395 | Pa×s | 968.88 | Joback Method |
| dvisc | 0.0000321 | Pa×s | 1028.36 | 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=U357976&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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