

Isophthalic acid, 2,3-dichlorophenyl pentyl ester

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|----------------------|---|
| Inchi: | InChI=1S/C19H18Cl2O4/c1-2-3-4-11-24-18(22)13-7-5-8-14(12-13)19(23)25-16-10-6-9-15 |
| InchiKey: | BJYLDRTWLNQMLO-UHFFFAOYSA-N |
| Formula: | C19H18Cl2O4 |
| SMILES: | CCCCCOC(=O)c1cccc(C(=O)Oc2cccc(Cl)c2Cl)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 |
| mvol | 270.410 | ml/mol | McGowan Method |
| pc | 1726.03 | kPa | Joback Method |
| rinpol | 2947.00 | | NIST Webbook |
| rinpol | 2947.00 | | NIST Webbook |
| tb | 929.86 | K | Joback Method |
| tc | 1163.73 | K | Joback Method |
| tf | 598.45 | K | Joback Method |
| vc | 1.030 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

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

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0002039 | Paxs | 653.69 | Joback Method |
| dvisc | 0.0001411 | Paxs | 708.92 | Joback Method |
| dvisc | 0.0001029 | Paxs | 764.15 | Joback Method |
| dvisc | 0.0000784 | Paxs | 819.39 | Joback Method |
| dvisc | 0.0000617 | Paxs | 874.62 | Joback Method |
| dvisc | 0.0000500 | Paxs | 929.86 | 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=U344527&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 |

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