

Succinic acid, 2,3-dichlorophenyl pent-4-en-1-yl ester

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|----------------------|---|
| Inchi: | InChI=1S/C15H16Cl2O4/c1-2-3-4-10-20-13(18)8-9-14(19)21-12-7-5-6-11(16)15(12)17/h2 |
| InchiKey: | VQMVLCVRDPKSDP-UHFFFAOYSA-N |
| Formula: | C15H16Cl2O4 |
| SMILES: | C=CCCCOC(=O)CCC(=O)Oc1cccc(Cl)c1Cl |
| Mol. weight [g/mol]: | 331.19 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -235.29 | kJ/mol | Joback Method |
| hf | -534.99 | kJ/mol | Joback Method |
| hfus | 40.56 | kJ/mol | Joback Method |
| hvap | 79.00 | kJ/mol | Joback Method |
| log10ws | -4.80 | | Crippen Method |
| logp | 4.188 | | Crippen Method |
| mvol | 233.510 | ml/mol | McGowan Method |
| pc | 1895.30 | kPa | Joback Method |
| rinpol | 2331.00 | | NIST Webbook |
| rinpol | 2331.00 | | NIST Webbook |
| tb | 803.36 | K | Joback Method |
| tc | 1017.75 | K | Joback Method |
| tf | 512.67 | K | Joback Method |
| vc | 0.894 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 617.36 | J/molxK | 803.36 | Joback Method |
| cpg | 629.29 | J/molxK | 839.09 | Joback Method |
| cpg | 640.29 | J/molxK | 874.82 | Joback Method |
| cpg | 650.37 | J/molxK | 910.55 | Joback Method |
| cpg | 659.54 | J/molxK | 946.29 | Joback Method |
| cpg | 667.82 | J/molxK | 982.02 | Joback Method |
| cpg | 675.22 | J/molxK | 1017.75 | Joback Method |
| dvisc | 0.0005863 | Paxs | 512.67 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003741 | Paxs | 561.12 | Joback Method |
| dvisc | 0.0002564 | Paxs | 609.57 | Joback Method |
| dvisc | 0.0001858 | Paxs | 658.01 | Joback Method |
| dvisc | 0.0001407 | Paxs | 706.46 | Joback Method |
| dvisc | 0.0001104 | Paxs | 754.91 | Joback Method |
| dvisc | 0.0000892 | Paxs | 803.36 | 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=U391074&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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