

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

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/h3-11,13-14,16-17,20-21
InchiKey: QAFGCOMEZMFPCE-ARJAWSKDSA-N
Formula: C15H16Cl2O4
SMILES: CCC=CCOC(=O)CCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 331.19

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -242.91 | kJ/mol | Joback Method |
| hf | -543.20 | kJ/mol | Joback Method |
| hfus | 42.04 | kJ/mol | Joback Method |
| hvap | 79.62 | kJ/mol | Joback Method |
| log10ws | -4.80 | | Crippen Method |
| logp | 4.188 | | Crippen Method |
| mcvol | 233.510 | ml/mol | McGowan Method |
| pc | 1911.91 | kPa | Joback Method |
| rinpol | 2350.00 | | NIST Webbook |
| rinpol | 2350.00 | | NIST Webbook |
| tb | 810.84 | K | Joback Method |
| tc | 1028.62 | K | Joback Method |
| tf | 509.35 | K | Joback Method |
| vc | 0.893 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 617.15 | J/molxK | 810.84 | Joback Method |
| cpg | 667.91 | J/molxK | 992.32 | Joback Method |
| cpg | 659.51 | J/molxK | 956.03 | Joback Method |
| cpg | 650.25 | J/molxK | 919.73 | Joback Method |
| cpg | 640.12 | J/molxK | 883.43 | Joback Method |
| cpg | 629.09 | J/molxK | 847.14 | Joback Method |
| cpg | 675.49 | J/molxK | 1028.62 | Joback Method |
| dvisc | 0.0000729 | Paxs | 810.84 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000908 | Paxs | 760.59 | Joback Method |
| dvisc | 0.0001169 | Paxs | 710.34 | Joback Method |
| dvisc | 0.0001562 | Paxs | 660.10 | Joback Method |
| dvisc | 0.0002191 | Paxs | 609.85 | Joback Method |
| dvisc | 0.0003265 | Paxs | 559.60 | Joback Method |
| dvisc | 0.0005264 | Paxs | 509.35 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.cheméo.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=U391268&Units=SI |

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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