

Succinic acid, 2,3-dichlorophenyl 2-hexyl ester

Inchi: InChI=1S/C16H20Cl2O4/c1-3-4-6-11(2)21-14(19)9-10-15(20)22-13-8-5-7-12(17)16(13)18
InchiKey: RYIWINSPCSNMMK-UHFFFAOYSA-N
Formula: C16H20Cl2O4
SMILES: CCCCC(C)OC(=O)CCC(=O)Oc1cccc(Cl)c1Cl
Mol. weight [g/mol]: 347.23

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -317.15 | kJ/mol | Joback Method |
| hf | -686.34 | kJ/mol | Joback Method |
| hfus | 40.90 | kJ/mol | Joback Method |
| hvap | 81.50 | kJ/mol | Joback Method |
| log10ws | -5.48 | | Crippen Method |
| logp | 4.801 | | Crippen Method |
| mvol | 251.900 | ml/mol | McGowan Method |
| pc | 1697.70 | kPa | Joback Method |
| rinpol | 2335.00 | | NIST Webbook |
| rinpol | 2335.00 | | NIST Webbook |
| tb | 829.12 | K | Joback Method |
| tc | 1042.01 | K | Joback Method |
| tf | 510.70 | K | Joback Method |
| vc | 0.964 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 699.46 | J/molxK | 829.12 | Joback Method |
| cpg | 712.39 | J/molxK | 864.60 | Joback Method |
| cpg | 724.28 | J/molxK | 900.08 | Joback Method |
| cpg | 735.15 | J/molxK | 935.56 | Joback Method |
| cpg | 745.00 | J/molxK | 971.05 | Joback Method |
| cpg | 753.85 | J/molxK | 1006.53 | Joback Method |
| cpg | 761.71 | J/molxK | 1042.01 | Joback Method |
| dvisc | 0.0005767 | Paxs | 510.70 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003401 | Paxs | 563.77 | Joback Method |
| dvisc | 0.0002196 | Paxs | 616.84 | Joback Method |
| dvisc | 0.0001520 | Paxs | 669.91 | Joback Method |
| dvisc | 0.0001111 | Paxs | 722.98 | Joback Method |
| dvisc | 0.0000847 | Paxs | 776.05 | Joback Method |
| dvisc | 0.0000669 | Paxs | 829.12 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U390692&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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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