

Succinic acid, decyl 2,3,5-trichlorophenyl ester

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|----------------------|-----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C20H27Cl3O4/c1-2-3-4-5-6-7-8-9-12-26-18(24)10-11-19(25)27-17-14-15(21)13 |
| InchiKey: | LQMDAUQYGDNOKV-UHFFFAOYSA-N |
| Formula: | C20H27Cl3O4 |
| SMILES: | CCCCCCCCCOC(=O)CCC(=O)Oc1cc(Cl)cc(Cl)c1Cl |
| Mol. weight [g/mol]: | 437.79 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -302.59 | kJ/mol | Joback Method |
| hf | -790.83 | kJ/mol | Joback Method |
| hfus | 58.59 | kJ/mol | Joback Method |
| hvap | 95.84 | kJ/mol | Joback Method |
| log10ws | -7.73 | | Crippen Method |
| logp | 7.016 | | Crippen Method |
| mvol | 320.500 | ml/mol | McGowan Method |
| pc | 1213.20 | kPa | Joback Method |
| rmpol | 2911.00 | | NIST Webbook |
| rmpol | 2911.00 | | NIST Webbook |
| tb | 963.49 | K | Joback Method |
| tc | 1182.62 | K | Joback Method |
| tf | 613.22 | K | Joback Method |
| vc | 1.242 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 950.93 | J/molxK | 963.49 | Joback Method |
| cpg | 1000.85 | J/molxK | 1146.10 | Joback Method |
| cpg | 993.26 | J/molxK | 1109.58 | Joback Method |
| cpg | 984.50 | J/molxK | 1073.05 | Joback Method |
| cpg | 974.53 | J/molxK | 1036.53 | Joback Method |
| cpg | 963.35 | J/molxK | 1000.01 | Joback Method |
| cpg | 1007.29 | J/molxK | 1182.62 | Joback Method |
| dvisc | 0.0000354 | Paxs | 963.49 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000442 | Paxs | 905.11 | Joback Method |
| dvisc | 0.0000570 | Paxs | 846.73 | Joback Method |
| dvisc | 0.0000762 | Paxs | 788.36 | Joback Method |
| dvisc | 0.0001068 | Paxs | 729.98 | Joback Method |
| dvisc | 0.0001586 | Paxs | 671.60 | Joback Method |
| dvisc | 0.0002540 | Paxs | 613.22 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U349615&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

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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