

Succinic acid, di(2,3,6-trichlorophenyl) ester

Inchi: InChI=1S/C16H8Cl6O4/c17-7-1-3-9(19)15(13(7)21)25-11(23)5-6-12(24)26-16-10(20)4-2
InchiKey: ATCHWTIBPUOJAN-UHFFFAOYSA-N
Formula: C16H8Cl6O4
SMILES: O=C(CCC(=O)Oc1c(Cl)ccc(Cl)c1Cl)Oc1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]: 476.95

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -288.54 | kJ/mol | Joback Method |
| hf | -553.37 | kJ/mol | Joback Method |
| hfus | 53.70 | kJ/mol | Joback Method |
| hvap | 104.36 | kJ/mol | Joback Method |
| log10ws | -7.86 | | Crippen Method |
| logp | 6.898 | | Crippen Method |
| mcvol | 277.100 | ml/mol | McGowan Method |
| pc | 1870.79 | kPa | Joback Method |
| rinpol | 3232.00 | | NIST Webbook |
| rinpol | 3232.00 | | NIST Webbook |
| tb | 1025.88 | K | Joback Method |
| tc | 1280.42 | K | Joback Method |
| tf | 721.88 | K | Joback Method |
| vc | 1.058 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 657.78 | J/molxK | 1025.88 | Joback Method |
| cpg | 662.72 | J/molxK | 1068.30 | Joback Method |
| cpg | 666.41 | J/molxK | 1110.73 | Joback Method |
| cpg | 668.86 | J/molxK | 1153.15 | Joback Method |
| cpg | 670.07 | J/molxK | 1195.57 | Joback Method |
| cpg | 670.03 | J/molxK | 1238.00 | Joback Method |
| cpg | 668.76 | J/molxK | 1280.42 | Joback Method |
| dvisc | 0.0001712 | Paxs | 721.88 | Joback Method |

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|-------|-----------|------|---------|---------------|
| dvisc | 0.0001264 | Paxs | 772.55 | Joback Method |
| dvisc | 0.0000968 | Paxs | 823.21 | Joback Method |
| dvisc | 0.0000765 | Paxs | 873.88 | Joback Method |
| dvisc | 0.0000621 | Paxs | 924.55 | Joback Method |
| dvisc | 0.0000514 | Paxs | 975.21 | Joback Method |
| dvisc | 0.0000434 | Paxs | 1025.88 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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=U349717&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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