

Sebacic acid, hexyl 2,3,5-trichlorophenyl ester

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|-----------------------------|-----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C22H31Cl3O4/c1-2-3-4-11-14-28-20(26)12-9-7-5-6-8-10-13-21(27)29-19-16-17 |
| InchiKey: | SWVVWSPESPFVAK-UHFFFAOYSA-N |
| Formula: | C22H31Cl3O4 |
| SMILES: | CCCCCOC(=O)CCCCCCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl |
| Mol. weight [g/mol]: | 465.84 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -285.75 | kJ/mol | Joback Method |
| hf | -832.11 | kJ/mol | Joback Method |
| hfus | 63.77 | kJ/mol | Joback Method |
| hvap | 100.29 | kJ/mol | Joback Method |
| log10ws | -8.56 | | Crippen Method |
| logp | 7.796 | | Crippen Method |
| mcvol | 348.680 | ml/mol | McGowan Method |
| pc | 1065.87 | kPa | Joback Method |
| rinqol | 3198.00 | | NIST Webbook |
| tb | 1009.25 | K | Joback Method |
| tc | 1235.70 | K | Joback Method |
| tf | 635.76 | K | Joback Method |
| vc | 1.355 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1069.88 | J/molxK | 1009.25 | Joback Method |
| cpg | 1120.23 | J/molxK | 1197.96 | Joback Method |
| cpg | 1112.81 | J/molxK | 1160.22 | Joback Method |
| cpg | 1104.10 | J/molxK | 1122.48 | Joback Method |
| cpg | 1094.07 | J/molxK | 1084.73 | Joback Method |
| cpg | 1082.67 | J/molxK | 1046.99 | Joback Method |
| cpg | 1126.38 | J/molxK | 1235.70 | Joback Method |
| dvisc | 0.0000261 | Paxs | 1009.25 | Joback Method |
| dvisc | 0.0000328 | Paxs | 947.00 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000426 | Paxs | 884.75 | Joback Method |
| dvisc | 0.0000575 | Paxs | 822.50 | Joback Method |
| dvisc | 0.0000815 | Paxs | 760.26 | Joback Method |
| dvisc | 0.0001231 | Paxs | 698.01 | Joback Method |
| dvisc | 0.0002015 | Paxs | 635.76 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U355201&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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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