

Succinic acid, dec-2-yl 4-octyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C22H42O4/c1-5-8-10-11-12-13-15-19(4)25-21(23)17-18-22(24)26-20(14-7-3)1 |
| InchiKey: | KZTYPXRSAMAKNG-UHFFFAOYSA-N |
| Formula: | C22H42O4 |
| SMILES: | CCCCCCCCC(C)OC(=O)CCC(=O)OC(CCC)CCCC |
| Mol. weight [g/mol]: | 370.57 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -338.36 | kJ/mol | Joback Method |
| hf | -997.57 | kJ/mol | Joback Method |
| hfus | 51.26 | kJ/mol | Joback Method |
| hvap | 82.10 | kJ/mol | Joback Method |
| log10ws | -6.98 | | Crippen Method |
| logp | 6.351 | | Crippen Method |
| mvol | 335.720 | ml/mol | McGowan Method |
| pc | 963.27 | kPa | Joback Method |
| rinpol | 2317.00 | | NIST Webbook |
| rinpol | 2317.00 | | NIST Webbook |
| tb | 854.46 | K | Joback Method |
| tc | 1046.57 | K | Joback Method |
| tf | 452.02 | K | Joback Method |
| vc | 1.304 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1092.98 | J/molxK | 854.46 | Joback Method |
| cpg | 1112.15 | J/molxK | 886.48 | Joback Method |
| cpg | 1130.10 | J/molxK | 918.50 | Joback Method |
| cpg | 1146.85 | J/molxK | 950.51 | Joback Method |
| cpg | 1162.43 | J/molxK | 982.53 | Joback Method |
| cpg | 1176.86 | J/molxK | 1014.55 | Joback Method |
| cpg | 1190.16 | J/molxK | 1046.57 | Joback Method |
| dvisc | 0.0009298 | Paxs | 452.02 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003731 | Paxs | 519.09 | Joback Method |
| dvisc | 0.0001845 | Paxs | 586.17 | Joback Method |
| dvisc | 0.0001055 | Paxs | 653.24 | Joback Method |
| dvisc | 0.0000669 | Paxs | 720.31 | Joback Method |
| dvisc | 0.0000458 | Paxs | 787.39 | Joback Method |
| dvisc | 0.0000333 | Paxs | 854.46 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U389566&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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