

Sebacic acid, 3-hexyl undecyl ester

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| Inchi: | InChI=1S/C27H52O4/c1-4-7-8-9-10-11-14-17-20-24-30-26(28)22-18-15-12-13-16-19-23- |
| InchiKey: | HDXIFXMGSLSCGD-UHFFFAOYSA-N |
| Formula: | C27H52O4 |
| SMILES: | CCCCCCCCCOC(=O)CCCCCCCC(=O)OC(CC)CCC |
| Mol. weight [g/mol]: | 440.70 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -293.82 | kJ/mol | Joback Method |
| hf | -1095.49 | kJ/mol | Joback Method |
| hfus | 67.74 | kJ/mol | Joback Method |
| hvap | 93.62 | kJ/mol | Joback Method |
| log10ws | -8.96 | | Crippen Method |
| logp | 8.303 | | Crippen Method |
| mcvol | 406.170 | ml/mol | McGowan Method |
| pc | 726.53 | kPa | Joback Method |
| rinsol | 2985.00 | | NIST Webbook |
| tb | 969.30 | K | Joback Method |
| tc | 1196.72 | K | Joback Method |
| tf | 523.37 | K | Joback Method |
| vc | 1.589 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1410.04 | J/molxK | 969.30 | Joback Method |
| cpg | 1431.86 | J/molxK | 1007.20 | Joback Method |
| cpg | 1451.85 | J/molxK | 1045.11 | Joback Method |
| cpg | 1470.06 | J/molxK | 1083.01 | Joback Method |
| cpg | 1486.55 | J/molxK | 1120.91 | Joback Method |
| cpg | 1501.39 | J/molxK | 1158.81 | Joback Method |
| cpg | 1514.63 | J/molxK | 1196.72 | Joback Method |
| dvisc | 0.0004080 | Paxs | 523.37 | Joback Method |
| dvisc | 0.0001723 | Paxs | 597.69 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000881 | Paxs | 672.01 | Joback Method |
| dvisc | 0.0000515 | Paxs | 746.34 | Joback Method |
| dvisc | 0.0000331 | Paxs | 820.66 | Joback Method |
| dvisc | 0.0000230 | Paxs | 894.98 | Joback Method |
| dvisc | 0.0000168 | Paxs | 969.30 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U355546&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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