

Sebacic acid, di(pent-4-en-2-yl) ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C20H34O4/c1-5-13-17(3)23-19(21)15-11-9-7-8-10-12-16-20(22)24-18(4)14-6-2 |
| InchiKey: | KRIHJLVYCYLOBE-UHFFFAOYSA-N |
| Formula: | C20H34O4 |
| SMILES: | <chem>C=CCC(C)OC(=O)CCCCCCCC(=O)OC(C)CC=C</chem> |
| Mol. weight [g/mol]: | 338.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -179.52 | kJ/mol | Joback Method |
| hf | -705.43 | kJ/mol | Joback Method |
| hfus | 43.52 | kJ/mol | Joback Method |
| hvap | 76.31 | kJ/mol | Joback Method |
| log10ws | -5.85 | | Crippen Method |
| logp | 5.123 | | Crippen Method |
| mcvol | 298.940 | ml/mol | McGowan Method |
| pc | 1152.22 | kPa | Joback Method |
| rinqol | 2222.00 | | NIST Webbook |
| tb | 802.06 | K | Joback Method |
| tc | 988.66 | K | Joback Method |
| tf | 425.96 | K | Joback Method |
| vc | 1.153 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 916.43 | J/molxK | 802.06 | Joback Method |
| cpg | 993.36 | J/molxK | 957.56 | Joback Method |
| cpg | 979.91 | J/molxK | 926.46 | Joback Method |
| cpg | 965.52 | J/molxK | 895.36 | Joback Method |
| cpg | 950.16 | J/molxK | 864.26 | Joback Method |
| cpg | 933.80 | J/molxK | 833.16 | Joback Method |
| cpg | 1005.90 | J/molxK | 988.66 | Joback Method |
| dvisc | 0.0000512 | Paxs | 802.06 | Joback Method |
| dvisc | 0.0000693 | Paxs | 739.38 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000994 | Paxs | 676.69 | Joback Method |
| dvisc | 0.0001534 | Paxs | 614.01 | Joback Method |
| dvisc | 0.0002613 | Paxs | 551.33 | Joback Method |
| dvisc | 0.0005101 | Paxs | 488.64 | Joback Method |
| dvisc | 0.0012128 | Paxs | 425.96 | Joback Method |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U355958&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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