

Sebacic acid, butyl 2-propylpentyl ester

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C22H42O4/c1-4-7-18-25-21(23)16-12-10-8-9-11-13-17-22(24)26-19-20(14-5-2 |
| InchiKey: | IMPAZGLULUMWAM-UHFFFAOYSA-N |
| Formula: | C22H42O4 |
| SMILES: | CCCCOC(=O)CCCCCCCC(=O)OCC(CCC)CCC |
| Mol. weight [g/mol]: | 370.57 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -335.92 | kJ/mol | Joback Method |
| hf | -992.29 | kJ/mol | Joback Method |
| hfus | 54.79 | kJ/mol | Joback Method |
| hvap | 82.49 | kJ/mol | Joback Method |
| log10ws | -6.51 | | Crippen Method |
| logp | 6.210 | | Crippen Method |
| mvol | 335.720 | ml/mol | McGowan Method |
| pc | 958.51 | kPa | Joback Method |
| rinpol | 2482.00 | | NIST Webbook |
| rinpol | 2482.00 | | NIST Webbook |
| tb | 854.90 | K | Joback Method |
| tc | 1046.82 | K | Joback Method |
| tf | 467.02 | K | Joback Method |
| vc | 1.310 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1092.52 | J/molxK | 854.90 | Joback Method |
| cpg | 1111.68 | J/molxK | 886.89 | Joback Method |
| cpg | 1129.63 | J/molxK | 918.87 | Joback Method |
| cpg | 1146.40 | J/molxK | 950.86 | Joback Method |
| cpg | 1162.01 | J/molxK | 982.84 | Joback Method |
| cpg | 1176.47 | J/molxK | 1014.83 | Joback Method |
| cpg | 1189.83 | J/molxK | 1046.82 | Joback Method |
| dvisc | 0.0007814 | Paxs | 467.02 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003435 | Paxs | 531.67 | Joback Method |
| dvisc | 0.0001805 | Paxs | 596.31 | Joback Method |
| dvisc | 0.0001075 | Paxs | 660.96 | Joback Method |
| dvisc | 0.0000703 | Paxs | 725.61 | Joback Method |
| dvisc | 0.0000492 | Paxs | 790.25 | Joback Method |
| dvisc | 0.0000364 | Paxs | 854.90 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U416209&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 |
| mccvol: | 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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