

Sebacic acid, heptyl nonyl ester

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| Inchi: | InChI=1S/C26H50O4/c1-3-5-7-9-12-16-20-24-30-26(28)22-18-14-11-10-13-17-21-25(27) |
| InchiKey: | XGYBGLORDMGBCU-UHFFFAOYSA-N |
| Formula: | C26H50O4 |
| SMILES: | CCCCCCCCCOC(=O)CCCCCCCCC(=O)OCCCCCCC |
| Mol. weight [g/mol]: | 426.67 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|----------|----------------------|----------------|
| gf | -299.80 | kJ/mol | Joback Method |
| hf | -1069.57 | kJ/mol | Joback Method |
| hfus | 68.67 | kJ/mol | Joback Method |
| hvap | 91.78 | kJ/mol | Joback Method |
| log10ws | -8.43 | | Crippen Method |
| logp | 7.915 | | Crippen Method |
| mvol | 392.080 | ml/mol | McGowan Method |
| pc | 762.26 | kPa | Joback Method |
| rinpol | 3028.00 | | NIST Webbook |
| rinpol | 3028.00 | | NIST Webbook |
| tb | 946.86 | K | Joback Method |
| tc | 1166.44 | K | Joback Method |
| tf | 527.10 | K | Joback Method |
| vc | 1.540 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1345.23 | J/molxK | 946.86 | Joback Method |
| cpg | 1366.62 | J/molxK | 983.46 | Joback Method |
| cpg | 1386.33 | J/molxK | 1020.05 | Joback Method |
| cpg | 1404.40 | J/molxK | 1056.65 | Joback Method |
| cpg | 1420.89 | J/molxK | 1093.25 | Joback Method |
| cpg | 1435.85 | J/molxK | 1129.84 | Joback Method |
| cpg | 1449.33 | J/molxK | 1166.44 | Joback Method |
| dvisc | 0.0004085 | Paxs | 527.10 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0001878 | Paxs | 597.06 | Joback Method |
| dvisc | 0.0001016 | Paxs | 667.02 | Joback Method |
| dvisc | 0.0000618 | Paxs | 736.98 | Joback Method |
| dvisc | 0.0000410 | Paxs | 806.94 | Joback Method |
| dvisc | 0.0000290 | Paxs | 876.90 | Joback Method |
| dvisc | 0.0000216 | Paxs | 946.86 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U354265&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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