

Sebacic acid, isohexyl 2-methylbutyl ester

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|-----------------------------|----------------------------------------------------------------------------------|
| Inchi: | InChI=1S/C21H40O4/c1-5-19(4)17-25-21(23)15-11-9-7-6-8-10-14-20(22)24-16-12-13-18 |
| InchiKey: | LZNJYIKIMGFVFZ-UHFFFAOYSA-N |
| Formula: | C21H40O4 |
| SMILES: | CCC(C)COC(=O)CCCCCCCCC(=O)OCCCC(C)C |
| Mol. weight [g/mol]: | 356.54 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -346.78 | kJ/mol | Joback Method |
| hf | -976.93 | kJ/mol | Joback Method |
| hfus | 48.67 | kJ/mol | Joback Method |
| hvap | 79.88 | kJ/mol | Joback Method |
| log10ws | -5.85 | | Crippen Method |
| logp | 5.676 | | Crippen Method |
| mvol | 321.630 | ml/mol | McGowan Method |
| pc | 1023.34 | kPa | Joback Method |
| rinpol | 2449.00 | | NIST Webbook |
| rinpol | 2449.00 | | NIST Webbook |
| tb | 831.58 | K | Joback Method |
| tc | 1019.89 | K | Joback Method |
| tf | 440.75 | K | Joback Method |
| vc | 1.248 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1031.20 | J/molxK | 831.58 | Joback Method |
| cpg | 1113.87 | J/molxK | 988.51 | Joback Method |
| cpg | 1099.54 | J/molxK | 957.12 | Joback Method |
| cpg | 1084.13 | J/molxK | 925.74 | Joback Method |
| cpg | 1067.62 | J/molxK | 894.35 | Joback Method |
| cpg | 1049.98 | J/molxK | 862.97 | Joback Method |
| cpg | 1127.14 | J/molxK | 1019.89 | Joback Method |
| dvisc | 0.0000387 | Paxs | 831.58 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000532 | Paxs | 766.44 | Joback Method |
| dvisc | 0.0000774 | Paxs | 701.30 | Joback Method |
| dvisc | 0.0001217 | Paxs | 636.16 | Joback Method |
| dvisc | 0.0002123 | Paxs | 571.03 | Joback Method |
| dvisc | 0.0004270 | Paxs | 505.89 | Joback Method |
| dvisc | 0.0010562 | Paxs | 440.75 | 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=U354339&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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<https://www.chemeo.com/cid/28-802-0/Sebacic-acid-isoheptyl-2-methylbutyl-ester.pdf>

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