

Sebacic acid, octyl pent-4-enyl ester

| | |
|-----------------------------|--|
| Inchi: | InChI=1S/C23H42O4/c1-3-5-7-8-13-17-21-27-23(25)19-15-12-10-9-11-14-18-22(24)26-2 |
| InchiKey: | MIAVDUGNLUNDMI-UHFFFAOYSA-N |
| Formula: | C23H42O4 |
| SMILES: | C=CCCCOC(=O)CCCCCCCCC(=O)OCCCCCCCC |
| Mol. weight [g/mol]: | 382.58 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -237.22 | kJ/mol | Joback Method |
| hf | -882.22 | kJ/mol | Joback Method |
| hfus | 59.62 | kJ/mol | Joback Method |
| hvap | 84.43 | kJ/mol | Joback Method |
| log10ws | -7.03 | | Crippen Method |
| logp | 6.520 | | Crippen Method |
| mvol | 345.510 | ml/mol | McGowan Method |
| pc | 922.74 | kPa | Joback Method |
| rinpol | 2675.00 | | NIST Webbook |
| rinpol | 2675.00 | | NIST Webbook |
| tb | 874.90 | K | Joback Method |
| tc | 1071.16 | K | Joback Method |
| tf | 491.53 | K | Joback Method |
| vc | 1.353 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1126.08 | J/molxK | 874.90 | Joback Method |
| cpg | 1145.15 | J/molxK | 907.61 | Joback Method |
| cpg | 1162.98 | J/molxK | 940.32 | Joback Method |
| cpg | 1179.62 | J/molxK | 973.03 | Joback Method |
| cpg | 1195.08 | J/molxK | 1005.74 | Joback Method |
| cpg | 1209.40 | J/molxK | 1038.45 | Joback Method |
| cpg | 1222.62 | J/molxK | 1071.16 | Joback Method |
| dvisc | 0.0006079 | Paxs | 491.53 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002910 | Paxs | 555.42 | Joback Method |
| dvisc | 0.0001622 | Paxs | 619.32 | Joback Method |
| dvisc | 0.0001008 | Paxs | 683.22 | Joback Method |
| dvisc | 0.0000680 | Paxs | 747.11 | Joback Method |
| dvisc | 0.0000488 | Paxs | 811.01 | Joback Method |
| dvisc | 0.0000367 | Paxs | 874.90 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U355414&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|----------------------------|---|
| cp_g: | 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: | Log ₁₀ 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 |

Latest version available from:

<https://www.chemeo.com/cid/19-862-4/Sebacic-acid-octyl-pent-4-enyl-ester.pdf>

Generated by Cheméo on 2024-04-26 16:48:33.860747975 +0000 UTC m=+16439362.781325297.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.