

Fumaric acid, dec-4-enyl pentyl ester

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|-----------------------------|--|
| Inchi: | InChI=1S/C19H32O4/c1-3-5-7-8-9-10-11-13-17-23-19(21)15-14-18(20)22-16-12-6-4-2/h |
| InchiKey: | UJUMBRGHJAFKHF-ZNGCIPOTSA-N |
| Formula: | C19H32O4 |
| SMILES: | CCCCC=CCCCOC(=O)C=CC(=O)OCCCCC |
| Mol. weight [g/mol]: | 324.45 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -198.30 | kJ/mol | Joback Method |
| hf | -690.65 | kJ/mol | Joback Method |
| hfus | 50.94 | kJ/mol | Joback Method |
| hvap | 76.12 | kJ/mol | Joback Method |
| log10ws | -5.21 | | Crippen Method |
| logp | 4.736 | | Crippen Method |
| mvol | 284.850 | ml/mol | McGowan Method |
| pc | 1234.61 | kPa | Joback Method |
| rinpol | 2261.00 | | NIST Webbook |
| rinpol | 2261.00 | | NIST Webbook |
| tb | 795.02 | K | Joback Method |
| tc | 982.06 | K | Joback Method |
| tf | 438.05 | K | Joback Method |
| vc | 1.107 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 859.06 | J/molxK | 795.02 | Joback Method |
| cpg | 875.80 | J/molxK | 826.19 | Joback Method |
| cpg | 891.63 | J/molxK | 857.37 | Joback Method |
| cpg | 906.59 | J/molxK | 888.54 | Joback Method |
| cpg | 920.71 | J/molxK | 919.71 | Joback Method |
| cpg | 934.02 | J/molxK | 950.88 | Joback Method |
| cpg | 946.55 | J/molxK | 982.06 | Joback Method |
| dvisc | 0.0008079 | Paxs | 438.05 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003774 | Paxs | 497.55 | Joback Method |
| dvisc | 0.0002074 | Paxs | 557.04 | Joback Method |
| dvisc | 0.0001279 | Paxs | 616.53 | Joback Method |
| dvisc | 0.0000859 | Paxs | 676.03 | Joback Method |
| dvisc | 0.0000616 | Paxs | 735.52 | Joback Method |
| dvisc | 0.0000463 | Paxs | 795.02 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U348939&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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