

Fumaric acid, dec-4-enyl hexadecyl ester

Inchi: InChI=1S/C30H54O4/c1-3-5-7-9-11-13-14-15-16-17-18-20-22-24-28-34-30(32)26-25-29(31)
InchiKey: HPGVPOJYSBDRGF-WISIHWMRSA-N
Formula: C30H54O4
SMILES: CCCCCC=CCCCOC(=O)C=CC(=O)OCCCCCCCCCCCCCCCCC
Mol. weight [g/mol]: 478.75

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -105.68 | kJ/mol | Joback Method |
| hf | -917.69 | kJ/mol | Joback Method |
| hfus | 79.43 | kJ/mol | Joback Method |
| hvap | 100.60 | kJ/mol | Joback Method |
| log10ws | -9.81 | | Crippen Method |
| logp | 9.027 | | Crippen Method |
| mvol | 439.840 | ml/mol | McGowan Method |
| pc | 656.79 | kPa | Joback Method |
| rinpol | 3377.00 | | NIST Webbook |
| rinpol | 3377.00 | | NIST Webbook |
| tb | 1046.70 | K | Joback Method |
| tc | 1305.52 | K | Joback Method |
| tf | 562.02 | K | Joback Method |
| vc | 1.724 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1548.54 | J/molxK | 1046.70 | Joback Method |
| cpg | 1571.96 | J/molxK | 1089.84 | Joback Method |
| cpg | 1593.55 | J/molxK | 1132.97 | Joback Method |
| cpg | 1613.46 | J/molxK | 1176.11 | Joback Method |
| cpg | 1631.83 | J/molxK | 1219.25 | Joback Method |
| cpg | 1648.81 | J/molxK | 1262.38 | Joback Method |
| cpg | 1664.56 | J/molxK | 1305.52 | Joback Method |
| dvisc | 0.0002071 | Paxs | 562.02 | Joback Method |

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|-------|-----------|------|---------|---------------|
| dvisc | 0.0000881 | Paxs | 642.80 | Joback Method |
| dvisc | 0.0000453 | Paxs | 723.58 | Joback Method |
| dvisc | 0.0000267 | Paxs | 804.36 | Joback Method |
| dvisc | 0.0000173 | Paxs | 885.14 | Joback Method |
| dvisc | 0.0000120 | Paxs | 965.92 | Joback Method |
| dvisc | 0.0000089 | Paxs | 1046.70 | 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=U348950&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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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