

Myristic acid, 4-methoxyphenyl ester

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C21H34O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-21(22)24-20-17-15-19(23-2)16-18 |
| InchiKey: | BYCQJIJKYKHTRV-UHFFFAOYSA-N |
| Formula: | C21H34O3 |
| SMILES: | CCCCCCCCCCCCC(=O)Oc1ccc(OC)cc1 |
| Mol. weight [g/mol]: | 334.49 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -110.20 | kJ/mol | Joback Method |
| hf | -628.73 | kJ/mol | Joback Method |
| hfus | 47.77 | kJ/mol | Joback Method |
| hvap | 76.84 | kJ/mol | Joback Method |
| log10ws | -6.93 | | Crippen Method |
| logp | 6.302 | | Crippen Method |
| mcvol | 296.300 | ml/mol | McGowan Method |
| pc | 1198.13 | kPa | Joback Method |
| rinpol | 2592.00 | | NIST Webbook |
| tb | 810.25 | K | Joback Method |
| tc | 1002.94 | K | Joback Method |
| tf | 459.76 | K | Joback Method |
| vc | 1.145 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 916.24 | J/molxK | 810.25 | Joback Method |
| cpg | 995.58 | J/molxK | 970.82 | Joback Method |
| cpg | 981.83 | J/molxK | 938.71 | Joback Method |
| cpg | 967.05 | J/molxK | 906.59 | Joback Method |
| cpg | 951.20 | J/molxK | 874.48 | Joback Method |
| cpg | 934.27 | J/molxK | 842.36 | Joback Method |
| cpg | 1008.32 | J/molxK | 1002.94 | Joback Method |
| dvisc | 0.0000494 | Paxs | 810.25 | Joback Method |
| dvisc | 0.0000644 | Paxs | 751.84 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000878 | Paxs | 693.42 | Joback Method |
| dvisc | 0.0001266 | Paxs | 635.00 | Joback Method |
| dvisc | 0.0001967 | Paxs | 576.59 | Joback Method |
| dvisc | 0.0003374 | Paxs | 518.17 | Joback Method |
| dvisc | 0.0006638 | Paxs | 459.76 | 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=U357930&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.cheméo.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 |

Latest version available from:

<https://www.cheméo.com/cid/64-147-8/Myristic-acid-4-methoxyphenyl-ester.pdf>

Generated by Cheméo on 2024-04-19 20:44:25.413402591 +0000 UTC m=+15848714.333979902.

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