

(E)-1-(4-Hydroxy-3-methoxyphenyl)hexadec-3-en-

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|-----------------------------|--|
| Inchi: | InChI=1S/C23H36O3/c1-3-4-5-6-7-8-9-10-11-15-21(24)16-13-12-14-20-17-18-22(25)23(|
| InchiKey: | ZRRQCKQGNSJPPU-DTQAZKPQSA-N |
| Formula: | C23H36O3 |
| SMILES: | CCCCCCCCCCCC(=O)C=CCCc1ccc(O)c(OC)c1 |
| Mol. weight [g/mol]: | 360.53 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -62.76 | kJ/mol | Joback Method |
| hf | -597.88 | kJ/mol | Joback Method |
| hfus | 57.75 | kJ/mol | Joback Method |
| hvap | 91.86 | kJ/mol | Joback Method |
| log10ws | -6.94 | | Crippen Method |
| logp | 6.380 | | Crippen Method |
| mcvol | 320.180 | ml/mol | McGowan Method |
| pc | 1219.99 | kPa | Joback Method |
| rinpol | 2862.20 | | NIST Webbook |
| rinpol | 2862.20 | | NIST Webbook |
| tb | 918.37 | K | Joback Method |
| tc | 1128.58 | K | Joback Method |
| tf | 566.71 | K | Joback Method |
| vc | 1.185 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 1043.46 | J/molxK | 918.37 | Joback Method |
| cpg | 1125.60 | J/molxK | 1093.55 | Joback Method |
| cpg | 1110.34 | J/molxK | 1058.51 | Joback Method |
| cpg | 1094.58 | J/molxK | 1023.48 | Joback Method |
| cpg | 1078.25 | J/molxK | 988.44 | Joback Method |
| cpg | 1061.25 | J/molxK | 953.41 | Joback Method |
| cpg | 1140.49 | J/molxK | 1128.58 | Joback Method |
| dvisc | 0.0000017 | Paxs | 918.37 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000026 | Paxs | 859.76 | Joback Method |
| dvisc | 0.0000041 | Paxs | 801.15 | Joback Method |
| dvisc | 0.0000069 | Paxs | 742.54 | Joback Method |
| dvisc | 0.0000127 | Paxs | 683.93 | Joback Method |
| dvisc | 0.0000264 | Paxs | 625.32 | Joback Method |
| dvisc | 0.0000635 | Paxs | 566.71 | 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=U413120&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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