# o-Methoxybenzoic acid, hexadecyl ester

**Inchi:** InChI=1S/C24H40O3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-27-24(25)22-19-16-17-2
**InchiKey:** WRPCOUMTSOAWBK-UHFFFAOYSA-N
**Formula:** C24H40O3
**SMILES:** CCCCCCCCCCCCCCCCOC(=O)c1ccccc1OC
**Mol. weight [g/mol]:** 376.57
**CAS:** 111722-09-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -84.94 | kJ/mol | Joback Method |
| hf | -690.65 | kJ/mol | Joback Method |
| hfus | 55.54 | kJ/mol | Joback Method |
| hvap | 83.52 | kJ/mol | Joback Method |
| log10ws | -8.11 | | Crippen Method |
| logp | 7.333 | | Crippen Method |
| mcvol | 338.570 | ml/mol | McGowan Method |
| pc | 990.75 | kPa | Joback Method |
| rinpol | 2744.80 | | NIST Webbook |
| rinpol | 2744.80 | | NIST Webbook |
| tb | 878.89 | K | Joback Method |
| tc | 1077.89 | K | Joback Method |
| tf | 493.57 | K | Joback Method |
| vc | 1.313 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1099.37 | J/mol×K | 878.89 | Joback Method |
| cpg | 1181.02 | J/mol×K | 1044.73 | Joback Method |
| cpg | 1167.09 | J/mol×K | 1011.56 | Joback Method |
| cpg | 1152.00 | J/mol×K | 978.39 | Joback Method |
| cpg | 1135.70 | J/mol×K | 945.22 | Joback Method |
| cpg | 1118.17 | J/mol×K | 912.06 | Joback Method |
| cpg | 1193.81 | J/mol×K | 1077.89 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000324 | Pa×s | 878.89 | Joback Method |
| dvisc | 0.0000425 | Pa×s | 814.67 | Joback Method |
| dvisc | 0.0000586 | Pa×s | 750.45 | Joback Method |
| dvisc | 0.0000856 | Pa×s | 686.23 | Joback Method |
| dvisc | 0.0001353 | Pa×s | 622.01 | Joback Method |
| dvisc | 0.0002376 | Pa×s | 557.79 | Joback Method |
| dvisc | 0.0004833 | Pa×s | 493.57 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C111722099&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# Legend

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|---|---|
| **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 |