# Benzoic acid, 3-methoxy-, heptyl ester

**Other names:** m-Methoxybenzoic acid, heptyl ester
**Inchi:** InChI=1S/C15H22O3/c1-3-4-5-6-7-11-18-15(16)13-9-8-10-14(12-13)17-2/h8-10,12H,3-7,
**InchiKey:** NDQYJNNGAZICSH-UHFFFAOYSA-N
**Formula:** C15H22O3
**SMILES:** CCCCCCCOC(=O)c1cccc(OC)c1
**Mol. weight [g/mol]:** 250.33
**CAS:** 69833-40-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -160.72 | kJ/mol | Joback Method |
| hf | -504.89 | kJ/mol | Joback Method |
| hfus | 32.23 | kJ/mol | Joback Method |
| hvap | 63.49 | kJ/mol | Joback Method |
| log10ws | -4.35 | | Crippen Method |
| logp | 3.822 | | Crippen Method |
| mcvol | 211.760 | ml/mol | McGowan Method |
| pc | 1869.17 | kPa | Joback Method |
| rinpol | 1924.80 | | NIST Webbook |
| rinpol | 1924.80 | | NIST Webbook |
| tb | 672.97 | K | Joback Method |
| tc | 869.94 | K | Joback Method |
| tf | 392.14 | K | Joback Method |
| vc | 0.809 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 574.00 | J/mol×K | 672.97 | Joback Method |
| cpg | 590.26 | J/mol×K | 705.80 | Joback Method |
| cpg | 605.64 | J/mol×K | 738.63 | Joback Method |
| cpg | 620.13 | J/mol×K | 771.45 | Joback Method |
| cpg | 633.77 | J/mol×K | 804.28 | Joback Method |
| cpg | 646.54 | J/mol×K | 837.11 | Joback Method |

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|---|---|---|---|---|
| cpg | 658.47 | J/mol×K | 869.94 | Joback Method |
| dvisc | 0.0010931 | Pa×s | 392.14 | Joback Method |
| dvisc | 0.0006017 | Pa×s | 438.95 | Joback Method |
| dvisc | 0.0003716 | Pa×s | 485.75 | Joback Method |
| dvisc | 0.0002498 | Pa×s | 532.56 | Joback Method |
| dvisc | 0.0001790 | Pa×s | 579.36 | Joback Method |
| dvisc | 0.0001349 | Pa×s | 626.17 | Joback Method |
| dvisc | 0.0001057 | Pa×s | 672.97 | Joback Method |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C69833405&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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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