# 6-Methoxythymyl isobutyrate

**Inchi:** InChI=1S/C16H24O3/c1-10(2)7-16(17)19-15-8-12(5)14(18-6)9-13(15)11(3)4/h8-11H,7H2
**InchiKey:** OPDWBYDWJIWHMN-UHFFFAOYSA-N
**Formula:** C16H24O3
**SMILES:** COc1cc(C(C)C)c(OC(=O)CC(C)C)cc1C
**Mol. weight [g/mol]:** 264.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -176.44 | kJ/mol | Joback Method |
| hf | -559.03 | kJ/mol | Joback Method |
| hfus | 27.00 | kJ/mol | Joback Method |
| hvap | 66.26 | kJ/mol | Joback Method |
| log10ws | -4.58 | | Crippen Method |
| logp | 4.079 | | Crippen Method |
| mcvol | 225.850 | ml/mol | McGowan Method |
| pc | 1703.31 | kPa | Joback Method |
| rinpol | 1658.00 | | NIST Webbook |
| ripol | 1998.00 | | NIST Webbook |
| tb | 704.93 | K | Joback Method |
| tc | 907.94 | K | Joback Method |
| tf | 398.45 | K | Joback Method |
| vc | 0.854 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 628.41 | J/mol×K | 704.93 | Joback Method |
| cpg | 703.67 | J/mol×K | 874.11 | Joback Method |
| cpg | 690.53 | J/mol×K | 840.27 | Joback Method |
| cpg | 676.44 | J/mol×K | 806.44 | Joback Method |
| cpg | 661.39 | J/mol×K | 772.60 | Joback Method |
| cpg | 645.38 | J/mol×K | 738.77 | Joback Method |
| cpg | 715.86 | J/mol×K | 907.94 | Joback Method |
| dvisc | 0.0000801 | Pa×s | 704.93 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001030 | Pa×s | 653.85 | Joback Method |
| dvisc | 0.0001380 | Pa×s | 602.77 | Joback Method |
| dvisc | 0.0001954 | Pa×s | 551.69 | Joback Method |
| dvisc | 0.0002970 | Pa×s | 500.61 | Joback Method |
| dvisc | 0.0004963 | Pa×s | 449.53 | Joback Method |
| dvisc | 0.0009462 | Pa×s | 398.45 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R518319&Units=SI |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |