# Acetic acid, 3-(2-methoxyethyl)heptyl ester

**Inchi:** InChI=1S/C12H24O3/c1-4-5-6-12(7-9-14-3)8-10-15-11(2)13/h12H,4-10H2,1-3H3
**InchiKey:** QCVMWYFKFLVGKN-UHFFFAOYSA-N
**Formula:** C12H24O3
**SMILES:** CCCCC(CCOC)CCOC(C)=O
**Mol. weight [g/mol]:** 216.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -291.20 | kJ/mol | Joback Method |
| hf | -673.31 | kJ/mol | Joback Method |
| hfus | 27.29 | kJ/mol | Joback Method |
| hvap | 53.48 | kJ/mol | Joback Method |
| log10ws | -2.55 | | Crippen Method |
| logp | 2.783 | | Crippen Method |
| mcvol | 193.250 | ml/mol | McGowan Method |
| pc | 1837.26 | kPa | Joback Method |
| rinpol | 1450.00 | | NIST Webbook |
| rinpol | 1450.00 | | NIST Webbook |
| tb | 572.23 | K | Joback Method |
| tc | 744.65 | K | Joback Method |
| tf | 304.39 | K | Joback Method |
| vc | 0.744 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 492.37 | J/mol×K | 572.23 | Joback Method |
| cpg | 508.15 | J/mol×K | 600.97 | Joback Method |
| cpg | 523.31 | J/mol×K | 629.70 | Joback Method |
| cpg | 537.87 | J/mol×K | 658.44 | Joback Method |
| cpg | 551.82 | J/mol×K | 687.18 | Joback Method |
| cpg | 565.17 | J/mol×K | 715.92 | Joback Method |
| cpg | 577.91 | J/mol×K | 744.65 | Joback Method |
| dvisc | 0.0029000 | Pa×s | 304.39 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0012682 | Pa×s | 349.03 | Joback Method |
| dvisc | 0.0006690 | Pa×s | 393.67 | Joback Method |
| dvisc | 0.0004020 | Pa×s | 438.31 | Joback Method |
| dvisc | 0.0002654 | Pa×s | 482.95 | Joback Method |
| dvisc | 0.0001880 | Pa×s | 527.59 | Joback Method |
| dvisc | 0.0001405 | Pa×s | 572.23 | 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=U368697&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 |