# Octadecanoic acid octadeca-9,12-dienyl ester, Z

**Inchi:** InChI=1S/C36H68O2/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-35-38-36(37)34-

**InchiKey:** GYQHSCDMKLFUOQ-GRAPOSQESA-N

**Formula:** C36H68O2

**SMILES:** CCCCCC=CCC=CCCCCCCCCOC(=O)CCCCCCCCCCCCCCCCC

**Mol. weight [g/mol]:** 532.92

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 178.76 | kJ/mol | Joback Method |
| hf | -796.73 | kJ/mol | Joback Method |
| hfus | 92.19 | kJ/mol | Joback Method |
| hvap | 104.80 | kJ/mol | Joback Method |
| log10ws | -13.46 | | Crippen Method |
| logp | 12.605 | | Crippen Method |
| mcvol | 516.940 | ml/mol | McGowan Method |
| pc | 488.60 | kPa | Joback Method |
| rinpol | 3717.06 | | NIST Webbook |
| rinpol | 3717.06 | | NIST Webbook |
| tb | 1107.69 | K | Joback Method |
| tc | 1426.10 | K | Joback Method |
| tf | 557.48 | K | Joback Method |
| vc | 2.035 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1899.39 | J/mol×K | 1107.69 | Joback Method |
| cpg | 1932.72 | J/mol×K | 1160.76 | Joback Method |
| cpg | 1963.73 | J/mol×K | 1213.83 | Joback Method |
| cpg | 1992.82 | J/mol×K | 1266.90 | Joback Method |
| cpg | 2020.40 | J/mol×K | 1319.96 | Joback Method |
| cpg | 2046.86 | J/mol×K | 1373.03 | Joback Method |
| cpg | 2072.61 | J/mol×K | 1426.10 | Joback Method |
| dvisc | 0.0001798 | Pa×s | 557.48 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000649 | Pa×s | 649.18 | Joback Method |
| dvisc | 0.0000301 | Pa×s | 740.88 | Joback Method |
| dvisc | 0.0000166 | Pa×s | 832.59 | Joback Method |
| dvisc | 0.0000103 | Pa×s | 924.29 | Joback Method |
| dvisc | 0.0000069 | Pa×s | 1015.99 | Joback Method |
| dvisc | 0.0000050 | Pa×s | 1107.69 | Joback Method |

# Sources

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|---|---|
| **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=R437097&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |