# Valeric acid, octyl ester

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|---|---|
| **Other names:** | Octyl pentanoate |
| | Pentanoic acid, octyl ester |
| | octyl valerate |
| **Inchi:** | InChI=1S/C13H26O2/c1-3-5-7-8-9-10-12-15-13(14)11-6-4-2/h3-12H2,1-2H3 |
| **InchiKey:** | OUYCCOBIJYUMAK-UHFFFAOYSA-N |
| **Formula:** | C13H26O2 |
| **SMILES:** | CCCCCCCCOC(=O)CCCC |
| **Mol. weight [g/mol]:** | 214.35 |
| **CAS:** | 5451-85-4 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.7296 | | Cheméo Relay (1.0) |
| gf | -175.34 | kJ/mol | Joback Method |
| hf | -631.34 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 32.21 | kJ/mol | Joback Method |
| hvap | 66.63 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.47 | eV | Cheméo Relay (1.0) |
| log10ws | -4.35 | | Cheméo Relay (1.0) |
| logp | 4.080 | | Crippen Method |
| mcvol | 201.470 | ml/mol | McGowan Method |
| pc | 1707.53 | kPa | Joback Method |
| tb | 522.50 | K | Cheméo Relay (1.0) |
| tc | 699.98 | K | Cheméo Relay (1.0) |
| tf | 236.44 | K | Cheméo Relay (1.0) |
| vc | 0.784 | m3/kmol | Cheméo Relay (1.0) |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 514.80 | J/mol×K | 573.13 | Joback Method |
| cpg | 531.11 | J/mol×K | 601.26 | Joback Method |
| cpg | 546.77 | J/mol×K | 629.39 | Joback Method |
| cpg | 561.79 | J/mol×K | 657.52 | Joback Method |

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|---|---|---|---|---|
| cpg | 576.19 | J/mol×K | 685.66 | Joback Method |
| cpg | 589.97 | J/mol×K | 713.79 | Joback Method |
| cpg | 603.14 | J/mol×K | 741.92 | Joback Method |
| dvisc | 0.0029408 | Pa×s | 308.43 | Joback Method |
| dvisc | 0.0013589 | Pa×s | 352.55 | Joback Method |
| dvisc | 0.0007456 | Pa×s | 396.66 | Joback Method |
| dvisc | 0.0004613 | Pa×s | 440.78 | Joback Method |
| dvisc | 0.0003115 | Pa×s | 484.90 | Joback Method |
| dvisc | 0.0002245 | Pa×s | 529.01 | Joback Method |
| dvisc | 0.0001702 | Pa×s | 573.13 | Joback Method |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.51157e+01 |
| Coeff. B | -4.67070e+03 |
| Coeff. C | -8.98100e+01 |
| Temperature range (K), min. | 404.80 |
| Temperature range (K), max. | 566.21 |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**Cheméo Relay (1.0):**

**The Yaws Handbook of Vapor Pressure:** https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

**KDB:** https://www.cheric.org/files/research/kdb/mol/mol1131.mol

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Cheméo Relay (1.0, beta):**

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C5451854&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

| | |
|---|---|
| **af:** | Acentric Factor |
| **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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |