# Eicosyl 3-methylpentanoate

**Inchi:** InChI=1S/C26H52O2/c1-4-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-28-26(2
**InchiKey:** RBNMPYXREKUVEQ-UHFFFAOYSA-N
**Formula:** C26H52O2
**SMILES:** CCCCCCCCCCCCCCCCCCCCCOC(=O)CC(C)CC
**Mol. weight [g/mol]:** 396.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -68.32 | kJ/mol | Joback Method |
| hf | -830.05 | kJ/mol | Joback Method |
| hfus | 62.36 | kJ/mol | Joback Method |
| hvap | 82.24 | kJ/mol | Joback Method |
| log10ws | -9.33 | | Crippen Method |
| logp | 9.008 | | Crippen Method |
| mcvol | 384.640 | ml/mol | McGowan Method |
| pc | 746.51 | kPa | Joback Method |
| rinpol | 2729.00 | | NIST Webbook |
| rinpol | 2729.00 | | NIST Webbook |
| tb | 870.13 | K | Joback Method |
| tc | 1066.30 | K | Joback Method |
| tf | 439.94 | K | Joback Method |
| vc | 1.510 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1285.77 | J/mol×K | 870.13 | Joback Method |
| cpg | 1308.62 | J/mol×K | 902.82 | Joback Method |
| cpg | 1330.12 | J/mol×K | 935.52 | Joback Method |
| cpg | 1350.31 | J/mol×K | 968.21 | Joback Method |
| cpg | 1369.26 | J/mol×K | 1000.91 | Joback Method |
| cpg | 1387.01 | J/mol×K | 1033.60 | Joback Method |
| cpg | 1403.60 | J/mol×K | 1066.30 | Joback Method |
| dvisc | 0.0009974 | Pa×s | 439.94 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003640 | Pa×s | 511.64 | Joback Method |
| dvisc | 0.0001702 | Pa×s | 583.34 | Joback Method |
| dvisc | 0.0000940 | Pa×s | 655.04 | Joback Method |
| dvisc | 0.0000583 | Pa×s | 726.73 | Joback Method |
| dvisc | 0.0000395 | Pa×s | 798.43 | Joback Method |
| dvisc | 0.0000285 | Pa×s | 870.13 | 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=R399252&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |