# Eicosanyl formate

**Inchi:** InChI=1S/C21H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-21-22/h2
**InchiKey:** XPSVNIWOCPFNFQ-UHFFFAOYSA-N
**Formula:** C21H42O2
**SMILES:** CCCCCCCCCCCCCCCCCCCCCOC=O
**Mol. weight [g/mol]:** 326.56

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -78.58 | kJ/mol | Joback Method |
| hf | -694.57 | kJ/mol | Joback Method |
| hfus | 53.62 | kJ/mol | Joback Method |
| hvap | 71.47 | kJ/mol | Joback Method |
| log10ws | -7.48 | | Crippen Method |
| logp | 7.201 | | Crippen Method |
| mcvol | 314.190 | ml/mol | McGowan Method |
| pc | 990.75 | kPa | Joback Method |
| rinpol | 2323.00 | | NIST Webbook |
| tb | 750.96 | K | Joback Method |
| tc | 922.75 | K | Joback Method |
| tf | 390.66 | K | Joback Method |
| vc | 1.246 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 967.84 | J/mol×K | 750.96 | Joback Method |
| cpg | 987.82 | J/mol×K | 779.59 | Joback Method |
| cpg | 1006.87 | J/mol×K | 808.22 | Joback Method |
| cpg | 1024.99 | J/mol×K | 836.86 | Joback Method |
| cpg | 1042.23 | J/mol×K | 865.49 | Joback Method |
| cpg | 1058.60 | J/mol×K | 894.12 | Joback Method |
| cpg | 1074.12 | J/mol×K | 922.75 | Joback Method |
| dvisc | 0.0017458 | Pa×s | 390.66 | Joback Method |
| dvisc | 0.0007187 | Pa×s | 450.71 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0003645 | Pa×s | 510.76 | Joback Method |
| dvisc | 0.0002133 | Pa×s | 570.81 | Joback Method |
| dvisc | 0.0001382 | Pa×s | 630.86 | Joback Method |
| dvisc | 0.0000965 | Pa×s | 690.91 | Joback Method |
| dvisc | 0.0000714 | Pa×s | 750.96 | Joback Method |

# Sources

| | |
|---|---|
| **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=R543003&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 |

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