# cis-5,8,11,14,17-Eicosapentaenoic acid, 4,4-dimethyloxazoline (dmox) derivative

**Inchi:** InChI=1S/C24H37NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-23-25-24(2,3

**InchiKey:** CQGLOTLOMZNEQB-AAQCHOMXSA-N

**Formula:** C24H37NO

**SMILES:** CCC=CCC=CCC=CCC=CCC=CCCCC1=NC(C)(C)CO1

**Mol. weight [g/mol]:** 355.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 634.35 | kJ/mol | Joback Method |
| hf | 108.41 | kJ/mol | Joback Method |
| hfus | 60.51 | kJ/mol | Joback Method |
| hvap | 79.59 | kJ/mol | Joback Method |
| log10ws | -7.89 | | Crippen Method |
| logp | 7.115 | | Crippen Method |
| mcvol | 328.210 | ml/mol | McGowan Method |
| pc | 1093.54 | kPa | Joback Method |
| rinpol | 2472.00 | | NIST Webbook |
| tb | 869.63 | K | Joback Method |
| tc | 1081.64 | K | Joback Method |
| tf | 481.03 | K | Joback Method |
| vc | 1.274 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1054.72 | J/mol×K | 869.63 | Joback Method |
| cpg | 1076.79 | J/mol×K | 904.97 | Joback Method |
| cpg | 1098.52 | J/mol×K | 940.30 | Joback Method |
| cpg | 1120.12 | J/mol×K | 975.64 | Joback Method |
| cpg | 1141.80 | J/mol×K | 1010.97 | Joback Method |
| cpg | 1163.74 | J/mol×K | 1046.31 | Joback Method |
| cpg | 1186.16 | J/mol×K | 1081.64 | 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=U333528&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 |
| **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 |