# cis-4,7,10,13,16,19-Docosahexaenoic acid, 4,4-dimethyloxazoline (dmox) derivative

**Inchi:** InChI=1S/C26H39NO/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23-25-27

**InchiKey:** BMZQUTWWFFVVNK-YNUSHXQLSA-N

**Formula:** C26H39NO

**SMILES:** CCC=CCC=CCC=CCC=CCC=CCC=CCCC1=NC(C)(C)CO1

**Mol. weight [g/mol]:** 381.59

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 731.41 | kJ/mol | Joback Method |
| hf | 184.35 | kJ/mol | Joback Method |
| hfus | 65.89 | kJ/mol | Joback Method |
| hvap | 84.00 | kJ/mol | Joback Method |
| log10ws | -8.58 | | Crippen Method |
| logp | 7.672 | | Crippen Method |
| mcvol | 352.090 | ml/mol | McGowan Method |
| pc | 998.91 | kPa | Joback Method |
| rinpol | 2655.80 | | NIST Webbook |
| tb | 919.55 | K | Joback Method |
| tc | 1136.41 | K | Joback Method |
| tf | 498.49 | K | Joback Method |
| vc | 1.367 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1155.40 | J/mol×K | 919.55 | Joback Method |
| cpg | 1178.87 | J/mol×K | 955.69 | Joback Method |
| cpg | 1202.33 | J/mol×K | 991.84 | Joback Method |
| cpg | 1226.01 | J/mol×K | 1027.98 | Joback Method |
| cpg | 1250.14 | J/mol×K | 1064.13 | Joback Method |
| cpg | 1274.97 | J/mol×K | 1100.27 | Joback Method |
| cpg | 1300.72 | J/mol×K | 1136.41 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U333234&Units=SI |

# 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 |