# 10-Undecynoic acid, 4,4-dimethyloxazoline (dmox) derivative

**Inchi:** InChI=1S/C15H25NO/c1-4-5-6-7-8-9-10-11-12-14-16-15(2,3)13-17-14/h1H,5-13H2,2-3H3

**InchiKey:** SIHYNDGTPLKOGL-UHFFFAOYSA-N

**Formula:** C15H25NO

**SMILES:** C#CCCCCCCCCC1=NC(C)(C)CO1

**Mol. weight [g/mol]:** 235.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 380.54 | kJ/mol | Joback Method |
| hf | -0.03 | kJ/mol | Joback Method |
| hfus | 39.17 | kJ/mol | Joback Method |
| hvap | 59.62 | kJ/mol | Joback Method |
| log10ws | -4.65 | | Crippen Method |
| logp | 3.948 | | Crippen Method |
| mcvol | 214.300 | ml/mol | McGowan Method |
| pc | 1937.24 | kPa | Joback Method |
| rinpol | 1637.80 | | NIST Webbook |
| tb | 633.03 | K | Joback Method |
| tc | 840.12 | K | Joback Method |
| tf | 451.97 | K | Joback Method |
| vc | 0.833 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 595.43 | J/mol×K | 633.03 | Joback Method |
| cpg | 614.72 | J/mol×K | 667.54 | Joback Method |
| cpg | 633.03 | J/mol×K | 702.06 | Joback Method |
| cpg | 650.47 | J/mol×K | 736.57 | Joback Method |
| cpg | 667.13 | J/mol×K | 771.09 | Joback Method |
| cpg | 683.13 | J/mol×K | 805.60 | Joback Method |
| cpg | 698.58 | J/mol×K | 840.12 | 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=U333574&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 |