# 4,8,12,16-Tetramethylheptadecan-4-olide

**Other names:** 5-Methyl-5-(4,8,12-trimethyltridecyl)dihydrofuran-2(3H)-one
**Inchi:** InChI=1S/C21H40O2/c1-17(2)9-6-10-18(3)11-7-12-19(4)13-8-15-21(5)16-14-20(22)23-21
**InchiKey:** LGWNRNDWDZHUNP-UHFFFAOYSA-N
**Formula:** C21H40O2
**SMILES:** CC(C)CCCC(C)CCCC(C)CCCC1(C)CCC(=O)O1
**Mol. weight [g/mol]:** 324.54
**CAS:** 96168-15-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -59.03 | kJ/mol | Joback Method |
| hf | -686.59 | kJ/mol | Joback Method |
| hfus | 34.70 | kJ/mol | Joback Method |
| hvap | 69.04 | kJ/mol | Joback Method |
| log10ws | -6.76 | | Crippen Method |
| logp | 6.521 | | Crippen Method |
| mcvol | 303.330 | ml/mol | McGowan Method |
| pc | 1142.12 | kPa | Joback Method |
| rinpol | 2364.20 | | NIST Webbook |
| rinpol | 2364.20 | | NIST Webbook |
| tb | 788.85 | K | Joback Method |
| tc | 986.27 | K | Joback Method |
| tf | 411.02 | K | Joback Method |
| vc | 1.161 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 981.94 | J/mol×K | 788.85 | Joback Method |
| cpg | 1004.50 | J/mol×K | 821.75 | Joback Method |
| cpg | 1026.17 | J/mol×K | 854.66 | Joback Method |
| cpg | 1047.03 | J/mol×K | 887.56 | Joback Method |
| cpg | 1067.20 | J/mol×K | 920.47 | Joback Method |
| cpg | 1086.76 | J/mol×K | 953.37 | Joback Method |

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|---|---|---|---|---|
| cpg | 1105.81 | J/mol×K | 986.27 | Joback Method |

# Sources

| | |
|---|---|
| **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=C96168159&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |