# 2-(2,4-Hexadiynylidene)-1,6-dioxaspiro[4,4]non-3-
# 2

**Inchi:** InChI=1S/C13H12O2/c1-2-3-4-5-7-12-8-10-13(15-12)9-6-11-14-13/h7-8,10H,6,9,11H2,1

**InchiKey:** WTRXKCNFPMTAJV-GHXNOFRVSA-N

**Formula:** C13H12O2

**SMILES:** CC#CC#CC=C1C=CC2(CCCO2)O1

**Mol. weight [g/mol]:** 200.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 454.78 | kJ/mol | Joback Method |
| hf | 265.46 | kJ/mol | Joback Method |
| hfus | 35.77 | kJ/mol | Joback Method |
| hvap | 58.44 | kJ/mol | Joback Method |
| log10ws | -3.63 | | Crippen Method |
| logp | 1.990 | | Crippen Method |
| mcvol | 158.250 | ml/mol | McGowan Method |
| pc | 3517.91 | kPa | Joback Method |
| rinpol | 1920.00 | | NIST Webbook |
| rinpol | 1920.00 | | NIST Webbook |
| tb | 605.74 | K | Joback Method |
| tc | 884.24 | K | Joback Method |
| tf | 566.19 | K | Joback Method |
| vc | 0.588 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 384.13 | J/mol×K | 605.74 | Joback Method |
| cpg | 400.74 | J/mol×K | 652.16 | Joback Method |
| cpg | 416.09 | J/mol×K | 698.57 | Joback Method |
| cpg | 430.51 | J/mol×K | 744.99 | Joback Method |
| cpg | 444.31 | J/mol×K | 791.41 | Joback Method |
| cpg | 457.79 | J/mol×K | 837.83 | Joback Method |
| cpg | 471.28 | J/mol×K | 884.24 | 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=R619695&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 |
| **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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