# 1,3-Dioxane, 2-ethyl-2methyl-4-pentyl, 2R,4R

**Inchi:** InChI=1S/C12H24O2/c1-4-6-7-8-11-9-10-13-12(3,5-2)14-11/h11H,4-10H2,1-3H3/t11-,12-
**InchiKey:** DURNOWZZDBQNIF-RYUDHWBXSA-N
**Formula:** C12H24O2
**SMILES:** CCCCCC1CCOC(C)(CC)O1
**Mol. weight [g/mol]:** 200.32

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -110.83 | kJ/mol | Joback Method |
| hf | -505.79 | kJ/mol | Joback Method |
| hfus | 29.40 | kJ/mol | Joback Method |
| hvap | 50.30 | kJ/mol | Joback Method |
| log10ws | -3.63 | | Crippen Method |
| logp | 3.498 | | Crippen Method |
| mcvol | 180.820 | ml/mol | McGowan Method |
| pc | 2121.68 | kPa | Joback Method |
| ripol | 1516.00 | | NIST Webbook |
| tb | 542.98 | K | Joback Method |
| tc | 740.89 | K | Joback Method |
| tf | 305.18 | K | Joback Method |
| vc | 0.679 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 466.39 | J/mol×K | 542.98 | Joback Method |
| cpg | 486.11 | J/mol×K | 575.96 | Joback Method |
| cpg | 504.78 | J/mol×K | 608.95 | Joback Method |
| cpg | 522.50 | J/mol×K | 641.93 | Joback Method |
| cpg | 539.34 | J/mol×K | 674.92 | Joback Method |
| cpg | 555.39 | J/mol×K | 707.90 | Joback Method |
| cpg | 570.74 | J/mol×K | 740.89 | 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=R191805&Units=SI |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |