# Tricyclo[4.2.1.02,5]non-3-ene,(1«alpha»,2«beta»,5

**Inchi:** InChI=1S/C13H20/c1-10-5-6-11(2,9-10)13(4)8-7-12(10,13)3/h7-8H,5-6,9H2,1-4H3/t10-,1
**InchiKey:** LQDIZUJFBWYDAZ-FNFFVJSTSA-N
**Formula:** C9H12
**SMILES:** CC12CCC(C)(C1)C1(C)C=CC21C
**Mol. weight [g/mol]:** 120.19
**CAS:** 16529-76-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 241.12 | kJ/mol | Joback Method |
| hf | 5.15 | kJ/mol | Joback Method |
| hfus | 0.93 | kJ/mol | Joback Method |
| hvap | 39.65 | kJ/mol | Joback Method |
| ie | 9.00 ± 0.05 | eV | NIST Webbook |
| log10ws | -3.84 | | Crippen Method |
| logp | 3.779 | | Crippen Method |
| mcvol | 157.150 | ml/mol | McGowan Method |
| pc | 2790.61 | kPa | Joback Method |
| tb | 512.51 | K | Joback Method |
| tc | 748.07 | K | Joback Method |
| tf | 382.21 | K | Joback Method |
| vc | 0.612 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 399.12 | J/mol×K | 512.51 | Joback Method |
| cpg | 419.50 | J/mol×K | 551.77 | Joback Method |
| cpg | 437.60 | J/mol×K | 591.03 | Joback Method |
| cpg | 454.00 | J/mol×K | 630.29 | Joback Method |
| cpg | 469.27 | J/mol×K | 669.55 | Joback Method |
| cpg | 484.01 | J/mol×K | 708.81 | Joback Method |
| cpg | 498.80 | J/mol×K | 748.07 | 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=C16529763&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 |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |