# Bicyclo[4.1.0]hepta-2,4-diene-7-carbonitrile, 7-phenyl-

**Inchi:** InChI=1S/C14H11N/c15-10-14(11-6-2-1-3-7-11)12-8-4-5-9-13(12)14/h1-9,12-13H
**InchiKey:** ZUEHDKCSXWCSAX-UHFFFAOYSA-N
**Formula:** C14H11N
**SMILES:** N#CC1(c2ccccc2)C2C=CC=CC21
**Mol. weight [g/mol]:** 193.24
**CAS:** 32777-15-4

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 468.71 | kJ/mol | Joback Method |
| hf | 319.02 | kJ/mol | Joback Method |
| hfus | 18.95 | kJ/mol | Joback Method |
| hvap | 58.63 | kJ/mol | Joback Method |
| log10ws | -3.34 | | Crippen Method |
| logp | 2.820 | | Crippen Method |
| mcvol | 155.420 | ml/mol | McGowan Method |
| pc | 2808.38 | kPa | Joback Method |
| tb | 660.12 | K | Joback Method |
| tc | 920.90 | K | Joback Method |
| tf | 392.49 | K | Joback Method |
| vc | 0.613 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 407.29 | J/mol×K | 660.12 | Joback Method |
| cpg | 422.19 | J/mol×K | 703.58 | Joback Method |
| cpg | 436.05 | J/mol×K | 747.05 | Joback Method |
| cpg | 449.20 | J/mol×K | 790.51 | Joback Method |
| cpg | 461.93 | J/mol×K | 833.97 | Joback Method |
| cpg | 474.55 | J/mol×K | 877.43 | Joback Method |
| cpg | 487.36 | J/mol×K | 920.90 | 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=C32777154&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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |