# Bicyclo[2.2.0]hexa-2,5-diene,1,2,3,4,5,6-hexafluoro

**Other names:** Perfluorobicyclo[2.2.0]hexa-2,5-diene
Hexafluorobicyclo[2.2.0]hexa-2,5-diene
Dewar hexafluorobenzene
Bicyclo[2.2.0]hexa-2,5-diene, hexafluoro-
**Inchi:** InChI=1S/C6F6/c7-1-2(8)6(12)4(10)3(9)5(1,6)11
**InchiKey:** NYGMLGNCZOOGFI-UHFFFAOYSA-N
**Formula:** C6F6
**SMILES:** FC1=C(F)C2(F)C(F)=C(F)C12F
**Mol. weight [g/mol]:** 186.05
**CAS:** 6733-01-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1037.30 | kJ/mol | Joback Method |
| hf | -1098.07 | kJ/mol | Joback Method |
| hfus | 14.34 | kJ/mol | Joback Method |
| hvap | 24.80 | kJ/mol | Joback Method |
| ie | 10.08 ± 0.05 | eV | NIST Webbook |
| ie | 10.40 | eV | NIST Webbook |
| ie | 10.40 ± 0.10 | eV | NIST Webbook |
| log10ws | -3.16 | | Crippen Method |
| logp | 2.731 | | Crippen Method |
| mcvol | 75.700 | ml/mol | McGowan Method |
| pc | 3452.08 | kPa | Joback Method |
| tb | 364.50 | K | Joback Method |
| tc | 525.14 | K | Joback Method |
| tf | 296.20 | K | Joback Method |
| vc | 0.361 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 160.76 | J/mol×K | 364.50 | Joback Method |
| cpg | 168.86 | J/mol×K | 391.27 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 176.00 | J/mol×K | 418.05 | Joback Method |
| cpg | 182.26 | J/mol×K | 444.82 | Joback Method |
| cpg | 187.73 | J/mol×K | 471.60 | Joback Method |
| cpg | 192.50 | J/mol×K | 498.37 | Joback Method |
| cpg | 196.67 | J/mol×K | 525.14 | Joback Method |

# Sources

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|---|---|
| **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=C6733013&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 |

Latest version available from:
https://www.chemeo.com/cid/63-407-0/Bicyclo-2-2-0-hexa-2-5-diene-1-2-3-4-5-6-hexafluoro.pdf
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