# Dibenzo[fg,st]hexacene

**Inchi:** InChI=1S/C32H18/c1-3-9-23-19(7-1)15-21-17-29-28-14-6-12-26-24-10-4-2-8-20(24)16-22
**InchiKey:** JEMVEIWDDNPRDI-UHFFFAOYSA-N
**Formula:** C32H18
**SMILES:** c1ccc2c(c1)cc1cc3c(cc4cc5ccccc5c5cccc3c45)c3cccc2c13
**Mol. weight [g/mol]:** 402.49
**CAS:** 313-97-3

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 1013.98 | kJ/mol | Joback Method |
| hf | 755.93 | kJ/mol | Joback Method |
| hfus | 52.45 | kJ/mol | Joback Method |
| hvap | 103.92 | kJ/mol | Joback Method |
| log10ws | -13.52 | | Crippen Method |
| logp | 9.197 | | Crippen Method |
| mcvol | 306.060 | ml/mol | McGowan Method |
| pc | 1707.53 | kPa | Joback Method |
| tb | 1113.28 | K | Joback Method |
| tc | 1393.93 | K | Joback Method |
| tf | 787.12 | K | Joback Method |
| vc | 1.204 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 980.19 | J/mol×K | 1113.28 | Joback Method |
| cpg | 1141.24 | J/mol×K | 1347.16 | Joback Method |
| cpg | 1101.51 | J/mol×K | 1300.38 | Joback Method |
| cpg | 1066.07 | J/mol×K | 1253.61 | Joback Method |
| cpg | 1034.40 | J/mol×K | 1206.83 | Joback Method |
| cpg | 1005.95 | J/mol×K | 1160.06 | Joback Method |
| cpg | 1185.80 | J/mol×K | 1393.93 | Joback Method |
| dvisc | 0.0110928 | Pa×s | 1113.28 | Joback Method |
| dvisc | 0.0114227 | Pa×s | 1058.92 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0117997 | Pa×s | 1004.56 | Joback Method |
| dvisc | 0.0122346 | Pa×s | 950.20 | Joback Method |
| dvisc | 0.0127414 | Pa×s | 895.84 | Joback Method |
| dvisc | 0.0133389 | Pa×s | 841.48 | Joback Method |
| dvisc | 0.0140531 | Pa×s | 787.12 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C313973&Units=SI |
| **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 |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |