# 5,2,1,6,3,4-[2,3]Butanediyl[1,4]diylidenedipentalen hexadecahydro-

**Other names:** Dodecahedrane
Pentagonal dodecahedrane

**Inchi:** InChI=1S/C20H20/c1-2-5-7-3(1)9-10-4(1)8-6(2)12-11(5)17-13(7)15(9)19-16(10)14(8)18(1

**InchiKey:** OOHPORRAEMMMCX-UHFFFAOYSA-N

**Formula:** C20H20

**SMILES:** C12C3C4C5C1C1C6C2C2C3C3C4C4C5C1C1C6C2C3C41

**Mol. weight [g/mol]:** 260.37

**CAS:** 4493-23-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 843.80 | kJ/mol | NIST Webbook |
| basg | 817.50 | kJ/mol | NIST Webbook |
| gf | 873.68 | kJ/mol | Joback Method |
| hf | 241.69 | kJ/mol | Joback Method |
| hfus | 63.98 | kJ/mol | Joback Method |
| hvap | 54.14 | kJ/mol | Joback Method |
| log10ws | -2.20 | | Crippen Method |
| logp | 2.460 | | Crippen Method |
| mcvol | 173.200 | ml/mol | McGowan Method |
| pc | 1841.99 | kPa | Joback Method |
| tb | 633.60 | K | Joback Method |
| tc | 833.77 | K | Joback Method |
| tf | 520.10 | K | Joback Method |
| vc | 0.777 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 666.22 | J/mol×K | 633.60 | Joback Method |
| cpg | 758.48 | J/mol×K | 800.41 | Joback Method |
| cpg | 741.77 | J/mol×K | 767.05 | Joback Method |
| cpg | 724.51 | J/mol×K | 733.68 | Joback Method |
| cpg | 706.38 | J/mol×K | 700.32 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 687.06 | J/mol×K | 666.96 | Joback Method |
| cpg | 774.97 | J/mol×K | 833.77 | Joback Method |
| dvisc | 399.6504679 | Pa×s | 633.60 | Joback Method |
| dvisc | 264.6826383 | Pa×s | 614.68 | Joback Method |
| dvisc | 170.7679261 | Pa×s | 595.77 | Joback Method |
| dvisc | 107.0544847 | Pa×s | 576.85 | Joback Method |
| dvisc | 65.0206799 | Pa×s | 557.93 | Joback Method |
| dvisc | 38.1327711 | Pa×s | 539.02 | Joback Method |
| dvisc | 21.5123048 | Pa×s | 520.10 | Joback Method |

# Sources

| | |
|---|---|
| **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=C4493236&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **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 |

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