# Dimer of «alpha»-phellandrene 2

**Inchi:** InChI=1S/C20H32/c1-14(2)16-7-8-19(6)17(13-16)18(5)9-11-20(19,12-10-18)15(3)4/h9,11
**InchiKey:** ANLKQZHORXQFDZ-UHFFFAOYSA-N
**Formula:** C20H32
**SMILES:** CC(C)C1=CC2C3(C)C=CC(C(C)C)(CC3)C2(C)CC1
**Mol. weight [g/mol]:** 272.47

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 284.70 | kJ/mol | Joback Method |
| hf | -137.30 | kJ/mol | Joback Method |
| hfus | 12.85 | kJ/mol | Joback Method |
| hvap | 57.08 | kJ/mol | Joback Method |
| log10ws | -6.14 | | Crippen Method |
| logp | 5.997 | | Crippen Method |
| mcvol | 251.480 | ml/mol | McGowan Method |
| pc | 1602.56 | kPa | Joback Method |
| rinpol | 1904.00 | | NIST Webbook |
| tb | 688.50 | K | Joback Method |
| tc | 919.87 | K | Joback Method |
| tf | 409.92 | K | Joback Method |
| vc | 0.956 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 755.37 | J/mol×K | 688.50 | Joback Method |
| cpg | 780.06 | J/mol×K | 727.06 | Joback Method |
| cpg | 804.04 | J/mol×K | 765.62 | Joback Method |
| cpg | 827.73 | J/mol×K | 804.18 | Joback Method |
| cpg | 851.58 | J/mol×K | 842.75 | Joback Method |
| cpg | 876.04 | J/mol×K | 881.31 | Joback Method |
| cpg | 901.53 | J/mol×K | 919.87 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R286394&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 |

# 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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |