# ((1R,4aR,4bR,10aR)-7-Isopropyl-1,4a-dimethyl-1,2

| | |
|---|---|
| **Other names:** | 1-Phenanthrenemethanol, 1,2,3,4,4a,4b,5,6,10,10a-decahydro-1,4a-dimethyl-7-(1-methylethyl)-, (1R,4aR,4bR,10aR)- |
| | Abietyl alcohol |
| | Podocarpa-7,13-dien-15-ol, 13-isopropyl- |
| | Abietinol |
| | Abietol |
| | [1R-(1«alpha»,4a«beta»,4b«alpha»,10a«alpha»)]-1,2,3,4,4a,4b,5,6,10,10a-decahydro-7- |
| **Inchi:** | InChI=1S/C20H32O/c1-14(2)15-6-8-17-16(12-15)7-9-18-19(3,13-21)10-5-11-20(17,18)4/ |
| **InchiKey:** | GQRUHVMVWNKUFW-WTGUMLROSA-N |
| **Formula:** | C20H32O |
| **SMILES:** | CC(C)C1=CC2=CCC3C(C)(CO)CCCC3(C)C2CC1 |
| **Mol. weight [g/mol]:** | 288.47 |
| **CAS:** | 666-84-2 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 121.98 | kJ/mol | Joback Method |
| hf | -323.28 | kJ/mol | Joback Method |
| hfus | 22.17 | kJ/mol | Joback Method |
| hvap | 76.30 | kJ/mol | Joback Method |
| log10ws | -5.64 | | Crippen Method |
| logp | 5.114 | | Crippen Method |
| mcvol | 257.350 | ml/mol | McGowan Method |
| pc | 1701.90 | kPa | Joback Method |
| rinpol | 2391.00 | | NIST Webbook |
| rinpol | 2391.00 | | NIST Webbook |
| rinpol | 2349.00 | | NIST Webbook |
| rinpol | 2349.00 | | NIST Webbook |
| rinpol | 2358.00 | | NIST Webbook |
| rinpol | 2389.00 | | NIST Webbook |
| rinpol | 2389.00 | | NIST Webbook |
| rinpol | 2391.00 | | NIST Webbook |
| tb | 794.40 | K | Joback Method |
| tc | 1012.23 | K | Joback Method |
| tf | 467.32 | K | Joback Method |
| vc | 0.967 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 843.75 | J/mol×K | 794.40 | Joback Method |
| cpg | 866.15 | J/mol×K | 830.71 | Joback Method |
| cpg | 888.26 | J/mol×K | 867.01 | Joback Method |
| cpg | 910.36 | J/mol×K | 903.32 | Joback Method |
| cpg | 932.70 | J/mol×K | 939.62 | Joback Method |
| cpg | 955.55 | J/mol×K | 975.93 | Joback Method |
| cpg | 979.16 | J/mol×K | 1012.23 | Joback Method |

# Sources

**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
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C666842&Units=SI

# 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