# Perhydrophenanthrene, 2A,4bB,8,8,10aB-pentamethyl-1B-(3-oxobutyl)

**Inchi:** InChI=1S/C23H40O/c1-16-8-11-20-22(5,18(16)10-9-17(2)24)15-12-19-21(3,4)13-7-14-23

**InchiKey:** XNAGUWARFHSTGQ-RTEXWSOPSA-N

**Formula:** C23H40O

**SMILES:** CC(=O)CCC1C(C)CCC2C1(C)CCC1C(C)(C)CCCC12C

**Mol. weight [g/mol]:** 332.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 88.30 | kJ/mol | Joback Method |
| hf | -478.67 | kJ/mol | Joback Method |
| hfus | 26.22 | kJ/mol | Joback Method |
| hvap | 69.45 | kJ/mol | Joback Method |
| log10ws | -6.72 | | Crippen Method |
| logp | 6.651 | | Crippen Method |
| mcvol | 303.920 | ml/mol | McGowan Method |
| pc | 1235.48 | kPa | Joback Method |
| rinpol | 2542.00 | | NIST Webbook |
| tb | 803.12 | K | Joback Method |
| tc | 1029.06 | K | Joback Method |
| tf | 489.86 | K | Joback Method |
| vc | 1.151 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1034.58 | J/mol×K | 803.12 | Joback Method |
| cpg | 1063.94 | J/mol×K | 840.78 | Joback Method |
| cpg | 1093.22 | J/mol×K | 878.43 | Joback Method |
| cpg | 1122.79 | J/mol×K | 916.09 | Joback Method |
| cpg | 1153.04 | J/mol×K | 953.75 | Joback Method |
| cpg | 1184.34 | J/mol×K | 991.40 | Joback Method |
| cpg | 1217.07 | J/mol×K | 1029.06 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R556920&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 |