# 3-Ethyl-8,8,11a-trimethyl-2,3,6,7,7a,8,9,10,11,11a-decahydro-1H-cyclopenta[a]chrys

**Inchi:** InChI=1S/C26H34/c1-5-17-7-8-19-18(17)9-10-21-20(19)11-13-23-22(21)12-14-24-25(2,3

**InchiKey:** BWXBAJIGBMHVQR-UHFFFAOYSA-N

**Formula:** C26H34

**SMILES:** CCC1CCc2c1ccc1c3c(ccc21)C1(C)CCCC(C)(C)C1CC3

**Mol. weight [g/mol]:** 346.55

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 487.94 | kJ/mol | Joback Method |
| hf | 17.97 | kJ/mol | Joback Method |
| hfus | 31.28 | kJ/mol | Joback Method |
| hvap | 77.51 | kJ/mol | Joback Method |
| log10ws | -8.67 | | Crippen Method |
| logp | 7.310 | | Crippen Method |
| mcvol | 301.400 | ml/mol | McGowan Method |
| pc | 1370.73 | kPa | Joback Method |
| rinpol | 3049.29 | | NIST Webbook |
| tb | 884.43 | K | Joback Method |
| tc | 1130.57 | K | Joback Method |
| tf | 582.32 | K | Joback Method |
| vc | 1.155 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1022.12 | J/mol×K | 884.43 | Joback Method |
| cpg | 1050.16 | J/mol×K | 925.45 | Joback Method |
| cpg | 1078.94 | J/mol×K | 966.48 | Joback Method |
| cpg | 1108.90 | J/mol×K | 1007.50 | Joback Method |
| cpg | 1140.51 | J/mol×K | 1048.53 | Joback Method |
| cpg | 1174.24 | J/mol×K | 1089.55 | Joback Method |
| cpg | 1210.53 | J/mol×K | 1130.57 | 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=R179716&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **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 |