# Dimyrcene I-a

**Inchi:** InChI=1S/C20H34/c1-6-20(14-8-10-18(4)5)15-12-19(13-16-20)11-7-9-17(2)3/h6,9-10,19H
**InchiKey:** ILNRJDGFLRCSOE-UHFFFAOYSA-N
**Formula:** C20H34
**SMILES:** C=CC1(CCC=C(C)C)CCC(CCC=C(C)C)CC1
**Mol. weight [g/mol]:** 274.48

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 359.95 | kJ/mol | Joback Method |
| hf | -66.62 | kJ/mol | Joback Method |
| hfus | 30.67 | kJ/mol | Joback Method |
| hvap | 58.49 | kJ/mol | Joback Method |
| log10ws | -7.17 | | Crippen Method |
| logp | 6.842 | | Crippen Method |
| mcvol | 268.900 | ml/mol | McGowan Method |
| pc | 1308.01 | kPa | Joback Method |
| ripol | 2144.00 | | NIST Webbook |
| ripol | 2149.00 | | NIST Webbook |
| tb | 676.88 | K | Joback Method |
| tc | 881.24 | K | Joback Method |
| tf | 302.36 | K | Joback Method |
| vc | 1.028 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 768.88 | J/mol×K | 676.88 | Joback Method |
| cpg | 792.30 | J/mol×K | 710.94 | Joback Method |
| cpg | 814.58 | J/mol×K | 745.00 | Joback Method |
| cpg | 835.86 | J/mol×K | 779.06 | Joback Method |
| cpg | 856.31 | J/mol×K | 813.12 | Joback Method |
| cpg | 876.05 | J/mol×K | 847.18 | Joback Method |
| cpg | 895.25 | J/mol×K | 881.24 | 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=R407175&Units=SI |

# 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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |