# Dehydroabietol ethyl benzoate

**Inchi:** InChI=1S/C28H36O2/c1-20(2)22-11-13-24-23(19-22)12-14-25-27(3,15-8-16-28(24,25)4)
**InchiKey:** PXADAXYXIKCJHQ-UHFFFAOYSA-N
**Formula:** C28H36O2
**SMILES:** CC(C)c1ccc2c(c1)CCC1C(C)(CCOC(=O)c3ccccc3)CCCC21C
**Mol. weight [g/mol]:** 404.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 232.69 | kJ/mol | Joback Method |
| hf | -277.79 | kJ/mol | Joback Method |
| hfus | 35.39 | kJ/mol | Joback Method |
| hvap | 90.12 | kJ/mol | Joback Method |
| log10ws | -8.06 | | Crippen Method |
| logp | 7.067 | | Crippen Method |
| mcvol | 343.580 | ml/mol | McGowan Method |
| pc | 1228.56 | kPa | Joback Method |
| rinpol | 3230.30 | | NIST Webbook |
| rinpol | 3230.30 | | NIST Webbook |
| tb | 997.04 | K | Joback Method |
| tc | 1243.96 | K | Joback Method |
| tf | 612.76 | K | Joback Method |
| vc | 1.298 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1211.02 | J/mol×K | 997.04 | Joback Method |
| cpg | 1241.08 | J/mol×K | 1038.19 | Joback Method |
| cpg | 1272.33 | J/mol×K | 1079.35 | Joback Method |
| cpg | 1305.15 | J/mol×K | 1120.50 | Joback Method |
| cpg | 1339.97 | J/mol×K | 1161.65 | Joback Method |
| cpg | 1377.17 | J/mol×K | 1202.81 | Joback Method |
| cpg | 1417.17 | J/mol×K | 1243.96 | Joback Method |

# Sources

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|---|---|
| **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=U414719&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |