# Phytol propionate

**Inchi:** InChI=1S/C23H44O2/c1-7-23(24)25-18-17-22(6)16-10-15-21(5)14-9-13-20(4)12-8-11-19
**InchiKey:** KJIHKRXSZYOFGU-IVNWLUGXSA-N
**Formula:** C23H44O2
**SMILES:** CCC(=O)OCC=C(C)CCCC(C)CCCC(C)CCCC(C)C
**Mol. weight [g/mol]:** 352.59

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -26.79 | kJ/mol | Joback Method |
| hf | -671.26 | kJ/mol | Joback Method |
| hfus | 46.44 | kJ/mol | Joback Method |
| hvap | 74.82 | kJ/mol | Joback Method |
| log10ws | -7.44 | | Crippen Method |
| logp | 7.325 | | Crippen Method |
| mcvol | 338.070 | ml/mol | McGowan Method |
| pc | 918.83 | kPa | Joback Method |
| rinpol | 2079.00 | | NIST Webbook |
| tb | 804.65 | K | Joback Method |
| tc | 989.69 | K | Joback Method |
| tf | 357.09 | K | Joback Method |
| vc | 1.310 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1069.77 | J/mol×K | 804.65 | Joback Method |
| cpg | 1090.59 | J/mol×K | 835.49 | Joback Method |
| cpg | 1110.32 | J/mol×K | 866.33 | Joback Method |
| cpg | 1128.99 | J/mol×K | 897.17 | Joback Method |
| cpg | 1146.65 | J/mol×K | 928.01 | Joback Method |
| cpg | 1163.35 | J/mol×K | 958.85 | Joback Method |
| cpg | 1179.12 | J/mol×K | 989.69 | 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=R572259&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 |