# Myraldyl acetate 1

**Inchi:** InChI=1S/C15H24O2/c1-12(2)6-4-7-14-8-5-9-15(10-14)11-17-13(3)16/h6,8,15H,4-5,7,9-1
**InchiKey:** IIUKCYITROTKFB-UHFFFAOYSA-N
**Formula:** C15H24O2
**SMILES:** CC(=O)OCC1CCC=C(CCC=C(C)C)C1
**Mol. weight [g/mol]:** 236.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -42.05 | kJ/mol | Joback Method |
| hf | -389.67 | kJ/mol | Joback Method |
| hfus | 28.95 | kJ/mol | Joback Method |
| hvap | 59.56 | kJ/mol | Joback Method |
| log10ws | -4.32 | | Crippen Method |
| logp | 4.022 | | Crippen Method |
| mcvol | 210.190 | ml/mol | McGowan Method |
| pc | 1843.58 | kPa | Joback Method |
| rinpol | 1704.00 | | NIST Webbook |
| rinpol | 1682.90 | | NIST Webbook |
| ripol | 2166.00 | | NIST Webbook |
| ripol | 2199.00 | | NIST Webbook |
| tb | 646.62 | K | Joback Method |
| tc | 851.38 | K | Joback Method |
| tf | 332.59 | K | Joback Method |
| vc | 0.799 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 571.56 | J/mol×K | 646.62 | Joback Method |
| cpg | 590.53 | J/mol×K | 680.75 | Joback Method |
| cpg | 608.43 | J/mol×K | 714.87 | Joback Method |
| cpg | 625.29 | J/mol×K | 749.00 | Joback Method |
| cpg | 641.15 | J/mol×K | 783.13 | Joback Method |
| cpg | 656.03 | J/mol×K | 817.26 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 669.97 | J/mol×K | 851.38 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R185865&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

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