# ETHANONE, 1-[4-(1-METHYL-2-PROPENYL)PHENYL]-

**Other names:** 1-[4-(1-Methyl-2-propenyl)phenyl]ethanone
**Inchi:** InChI=1S/C12H14O/c1-4-9(2)11-5-7-12(8-6-11)10(3)13/h4-9H,1H2,2-3H3
**InchiKey:** PGFYBSVJKSNEJQ-UHFFFAOYSA-N
**Formula:** C12H14O
**SMILES:** C=CC(C)c1ccc(C(C)=O)cc1
**Mol. weight [g/mol]:** 174.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| af | 0.4395 | | Cheméo Relay (1.0) |
| gf | 109.42 | kJ/mol | Joback Method |
| hf | -107.02 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 17.28 | kJ/mol | Joback Method |
| hvap | 70.67 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.86 | eV | Cheméo Relay (1.0) |
| log10ws | -3.46 | | Cheméo Relay (1.0) |
| logp | 3.179 | | Crippen Method |
| mcvol | 153.450 | ml/mol | McGowan Method |
| pc | 2654.29 | kPa | Joback Method |
| rinpol | 1883.00 | | NIST Webbook |
| tb | 531.57 | K | Cheméo Relay (1.0) |
| tc | 740.73 | K | Cheméo Relay (1.0) |
| tf | 299.46 | K | Cheméo Relay (1.0) |
| vc | 0.544 | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 348.98 | J/mol×K | 555.73 | Joback Method |
| cpg | 363.98 | J/mol×K | 592.10 | Joback Method |
| cpg | 378.05 | J/mol×K | 628.48 | Joback Method |
| cpg | 391.24 | J/mol×K | 664.85 | Joback Method |
| cpg | 403.57 | J/mol×K | 701.23 | Joback Method |
| cpg | 415.09 | J/mol×K | 737.60 | Joback Method |

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|---|---|---|---|---|
| cpg | 425.84 | J/mol×K | 773.97 | Joback Method |
| dvisc | 0.0027861 | Pa×s | 297.11 | Joback Method |
| dvisc | 0.0013837 | Pa×s | 340.21 | Joback Method |
| dvisc | 0.0008043 | Pa×s | 383.32 | Joback Method |
| dvisc | 0.0005217 | Pa×s | 426.42 | Joback Method |
| dvisc | 0.0003664 | Pa×s | 469.52 | Joback Method |
| dvisc | 0.0002731 | Pa×s | 512.63 | Joback Method |
| dvisc | 0.0002130 | Pa×s | 555.73 | Joback Method |

# Sources

**Cheméo Relay (1.0):**

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C109586494&Units=SI

**Joback Method:** https://en.wikipedia.org/wiki/Joback_method

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

**af:** Acentric Factor
**cpg:** Ideal gas heat capacity
**dvisc:** Dynamic viscosity
**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
**ie:** Ionization energy
**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