# Phenol, 3,4-dimethyl-, methylcarbamate

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|---|---|
| **Other names:** | Xylylcarb |
| | Carbamic acid, methyl-, 3,4-xylyl ester |
| | Meobal |
| | MPMC |
| | V 17004 |
| | 3,4-Dimethylphenyl methylcarbamate |
| | 3,4-Dimethylphenyl N-methylcarbamate |
| | 3,4-Xylyl methylcarbamate |
| | 3,4-Xylyl N-methylcarbamate |
| | Carbamic acid, N-methyl-, (3,4-dimethylphenyl) ester |
| | Methylcarbamic acid 3,4-xylyl ester |
| | S-1042 |
| | Xylecarb |
| | 3,4-Xylylester kyseliny methylkarbaminove |
| | Carbamic acid, 3,4-dimethylphenyl ester, N-methyl |
| | Phenol, 3,4-dimethyl-, 1-(N-methylcarbamate) |
| **Inchi:** | InChI=1S/C10H13NO2/c1-7-4-5-9(6-8(7)2)13-10(12)11-3/h4-6H,1-3H3,(H,11,12) |
| **InchiKey:** | WCJYTPVNMWIZCG-UHFFFAOYSA-N |
| **Formula:** | C10H13NO2 |
| **SMILES:** | CNC(=O)Oc1ccc(C)c(C)c1 |
| **Mol. weight [g/mol]:** | 179.22 |
| **CAS:** | 2425-10-7 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -18.06 | kJ/mol | Joback Method |
| hf | -227.47 | kJ/mol | Joback Method |
| hfus | 22.81 | kJ/mol | Joback Method |
| hvap | 57.05 | kJ/mol | Joback Method |
| log10ws | -2.90 | | Crippen Method |
| logp | 2.022 | | Crippen Method |
| mcvol | 145.420 | ml/mol | McGowan Method |
| pc | 3025.61 | kPa | Joback Method |
| rinpol | 1543.00 | | NIST Webbook |
| rinpol | 1536.00 | | NIST Webbook |
| ripol | 2132.00 | | NIST Webbook |
| ripol | 2132.00 | | NIST Webbook |

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|---|---|---|---|
| tb | 591.30 | K | Joback Method |
| tc | 805.99 | K | Joback Method |
| tf | 351.37 ± 0.20 | K | NIST Webbook |
| vc | 0.546 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 346.95 | J/mol×K | 591.30 | Joback Method |
| cpg | 360.01 | J/mol×K | 627.08 | Joback Method |
| cpg | 372.35 | J/mol×K | 662.86 | Joback Method |
| cpg | 383.98 | J/mol×K | 698.65 | Joback Method |
| cpg | 394.92 | J/mol×K | 734.43 | Joback Method |
| cpg | 405.16 | J/mol×K | 770.21 | Joback Method |
| cpg | 414.72 | J/mol×K | 805.99 | Joback Method |
| hfust | 24.97 | kJ/mol | 350.80 | NIST Webbook |
| hfust | 24.97 | kJ/mol | 350.80 | NIST Webbook |

# Sources

**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=C2425107&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
**hfust:** Enthalpy of fusion at a given temperature
**hvap:** Enthalpy of vaporization at standard conditions
**log10ws:** Log10 of Water solubility in mol/l

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|---|---|
| **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 |