

Formic acid, (4-methylphenyl)methyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C9H10O2/c1-8-2-4-9(5-3-8)6-11-7-10/h2-5,7H,6H2,1H3 |
| InchiKey: | MWCCNIVWHAWABQ-UHFFFAOYSA-N |
| Formula: | C9H10O2 |
| SMILES: | Cc1ccc(COC=O)cc1 |
| Mol. weight [g/mol]: | 150.17 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -76.84 | kJ/mol | Joback Method |
| hf | -221.83 | kJ/mol | Joback Method |
| hfus | 16.20 | kJ/mol | Joback Method |
| hvap | 47.70 | kJ/mol | Joback Method |
| log10ws | -2.11 | | Crippen Method |
| logp | 1.668 | | Crippen Method |
| mvol | 121.350 | ml/mol | McGowan Method |
| pc | 3423.86 | kPa | Joback Method |
| rinpol | 1199.00 | | NIST Webbook |
| tb | 508.06 | K | Joback Method |
| tc | 719.99 | K | Joback Method |
| tf | 294.36 | K | Joback Method |
| vc | 0.467 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 257.62 | J/molxK | 508.06 | Joback Method |
| cpg | 269.51 | J/molxK | 543.38 | Joback Method |
| cpg | 280.78 | J/molxK | 578.70 | Joback Method |
| cpg | 291.44 | J/molxK | 614.02 | Joback Method |
| cpg | 301.51 | J/molxK | 649.35 | Joback Method |
| cpg | 310.99 | J/molxK | 684.67 | Joback Method |
| cpg | 319.90 | J/molxK | 719.99 | Joback Method |
| dvisc | 0.0019322 | Paxs | 294.36 | Joback Method |
| dvisc | 0.0011334 | Paxs | 329.98 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0007377 | Paxs | 365.59 | Joback Method |
| dvisc | 0.0005181 | Paxs | 401.21 | Joback Method |
| dvisc | 0.0003855 | Paxs | 436.83 | Joback Method |
| dvisc | 0.0002999 | Paxs | 472.44 | Joback Method |
| dvisc | 0.0002417 | Paxs | 508.06 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U368937&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |

Legend

| | |
|-----------------|---|
| 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 |
| 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 |

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<https://www.chemeo.com/cid/21-431-9/Formic-acid-4-methylphenyl-methyl-ester.pdf>

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