

Formic acid, cis-4-methylcyclohexyl ester

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|-----------------------------|----------------------------------------------------------|
| Inchi: | InChI=1S/C8H14O2/c1-7-2-4-8(5-3-7)10-6-9/h6-8H,2-5H2,1H3 |
| InchiKey: | DZRDTGDYROJVPD-UHFFFAOYSA-N |
| Formula: | C8H14O2 |
| SMILES: | CC1CCC(OC=O)CC1 |
| Mol. weight [g/mol]: | 142.20 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -171.30 | kJ/mol | Joback Method |
| hf | -392.27 | kJ/mol | Joback Method |
| hfus | 12.86 | kJ/mol | Joback Method |
| hvap | 42.65 | kJ/mol | Joback Method |
| log10ws | -1.80 | | Crippen Method |
| logp | 1.738 | | Crippen Method |
| mvol | 120.160 | ml/mol | McGowan Method |
| pc | 3239.34 | kPa | Joback Method |
| rinpol | 1035.00 | | NIST Webbook |
| rinpol | 1035.00 | | NIST Webbook |
| tb | 468.40 | K | Joback Method |
| tc | 674.15 | K | Joback Method |
| tf | 247.29 | K | Joback Method |
| vc | 0.451 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 264.74 | J/molxK | 468.40 | Joback Method |
| cpg | 280.75 | J/molxK | 502.69 | Joback Method |
| cpg | 296.05 | J/molxK | 536.98 | Joback Method |
| cpg | 310.62 | J/molxK | 571.28 | Joback Method |
| cpg | 324.48 | J/molxK | 605.57 | Joback Method |
| cpg | 337.63 | J/molxK | 639.86 | Joback Method |
| cpg | 350.06 | J/molxK | 674.15 | Joback Method |
| dvisc | 0.0034215 | Paxs | 247.29 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0017716 | Paxs | 284.14 | Joback Method |
| dvisc | 0.0010669 | Paxs | 320.99 | Joback Method |
| dvisc | 0.0007133 | Paxs | 357.85 | Joback Method |
| dvisc | 0.0005141 | Paxs | 394.70 | Joback Method |
| dvisc | 0.0003919 | Paxs | 431.55 | Joback Method |
| dvisc | 0.0003117 | Paxs | 468.40 | Joback Method |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| 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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U368247&Units=SI |

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/91-836-3/Formic-acid-cis-4-methylcyclohexyl-ester.pdf>

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