

furfural acetal

Inchi: InChI=1S/C10H16O2/c1-3-11-10(12-4-2)9-7-5-6-8-9/h5-7,10H,3-4,8H2,1-2H3
InchiKey: MYMKNEUWNLGERL-UHFFFAOYSA-N
Formula: C10H16O2
SMILES: CCOC(OCC)C1=CC=CC1
Mol. weight [g/mol]: 168.23

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -84.57 | kJ/mol | Joback Method |
| hf | -334.54 | kJ/mol | Joback Method |
| hfus | 15.43 | kJ/mol | Joback Method |
| hvap | 44.10 | kJ/mol | Joback Method |
| log10ws | -2.39 | | Crippen Method |
| logp | 2.272 | | Crippen Method |
| mcvol | 144.040 | ml/mol | McGowan Method |
| pc | 2673.54 | kPa | Joback Method |
| ripol | 1663.00 | | NIST Webbook |
| ripol | 1663.00 | | NIST Webbook |
| tb | 495.85 | K | Joback Method |
| tc | 692.59 | K | Joback Method |
| tf | 261.10 | K | Joback Method |
| vc | 0.539 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 322.82 | J/mol×K | 495.85 | Joback Method |
| cpg | 337.81 | J/mol×K | 528.64 | Joback Method |
| cpg | 352.13 | J/mol×K | 561.43 | Joback Method |
| cpg | 365.78 | J/mol×K | 594.22 | Joback Method |
| cpg | 378.78 | J/mol×K | 627.01 | Joback Method |
| cpg | 391.13 | J/mol×K | 659.80 | Joback Method |
| cpg | 402.85 | J/mol×K | 692.59 | Joback Method |
| dvisc | 0.0026405 | Paxs | 261.10 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0012806 | Paxs | 300.23 | Joback Method |
| dvisc | 0.0007339 | Paxs | 339.35 | Joback Method |
| dvisc | 0.0004718 | Paxs | 378.48 | Joback Method |
| dvisc | 0.0003296 | Paxs | 417.60 | Joback Method |
| dvisc | 0.0002448 | Paxs | 456.73 | Joback Method |
| dvisc | 0.0001905 | Paxs | 495.85 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R340859&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

| | |
|----------------------------|---|
| cp_g: | 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 |
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| log₁₀ws: | Log ₁₀ of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| ripol: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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