

Bicyclo(2.2.1)heptane-2-carboxylic acid, endo-

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|-----------------------------|---|
| Inchi: | InChI=1S/C8H12O2/c9-8(10)7-4-5-1-2-6(7)3-5/h5-7H,1-4H2,(H,9,10)/t5?,6?,7-/m0/s1 |
| InchiKey: | JESWDXIHOJGWBP-AHXFUIDQSA-N |
| Formula: | C8H12O2 |
| SMILES: | O=C(O)C1CC2CCC1C2 |
| Mol. weight [g/mol]: | 140.18 |
| CAS: | 934-28-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|---------|----------------|
| gf | -147.57 | kJ/mol | Joback Method |
| hf | -354.16 | kJ/mol | Joback Method |
| hfus | 17.40 | kJ/mol | Joback Method |
| hvap | 56.52 | kJ/mol | Joback Method |
| log10ws | -1.33 | | Crippen Method |
| logp | 1.507 | | Crippen Method |
| mcvol | 109.300 | ml/mol | McGowan Method |
| pc | 4010.84 | kPa | Joback Method |
| tb | 541.57 | K | Joback Method |
| tc | 741.38 | K | Joback Method |
| tf | 332.00 ± 1.00 | K | NIST Webbook |
| vc | 0.413 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 281.77 | J/molxK | 541.57 | Joback Method |
| cpg | 294.95 | J/molxK | 574.87 | Joback Method |
| cpg | 307.30 | J/molxK | 608.17 | Joback Method |
| cpg | 318.88 | J/molxK | 641.48 | Joback Method |
| cpg | 329.72 | J/molxK | 674.78 | Joback Method |
| cpg | 339.89 | J/molxK | 708.08 | Joback Method |
| cpg | 349.43 | J/molxK | 741.38 | Joback Method |
| dvisc | 0.0071130 | Paxs | 318.79 | Joback Method |
| dvisc | 0.0037411 | Paxs | 355.92 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0022216 | Paxs | 393.05 | Joback Method |
| dvisc | 0.0014435 | Paxs | 430.18 | Joback Method |
| dvisc | 0.0010044 | Paxs | 467.31 | Joback Method |
| dvisc | 0.0007372 | Paxs | 504.44 | Joback Method |
| dvisc | 0.0005645 | Paxs | 541.57 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|---------------|------|----------------|--------------|
| tbrp | 381.50 ± 0.50 | K | 0.30 | NIST Webbook |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C934281&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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |

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 |
| tb: | Normal Boiling Point Temperature |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |

vc: Critical Volume

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