

# 1,4-Dioxo-8-azaspiro(4.5)decane

|                      |                                                                                                                                 |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Piperidone-4-ethyleneketal<br>4-Piperidone ethylene ketal<br>1,4-Dioxo-8-azaspiro[4,5]decane<br>1,4-dioxo-8-azaspiro[4.5]decane |
| Inchi:               | InChI=1S/C7H13NO2/c1-3-8-4-2-7(1)9-5-6-10-7/h8H,1-6H2                                                                           |
| InchiKey:            | KPKNTUUIEVXMOH-UHFFFAOYSA-N                                                                                                     |
| Formula:             | C7H13NO2                                                                                                                        |
| SMILES:              | C1CC2(CCN1)OCCO2                                                                                                                |
| Mol. weight [g/mol]: | 143.19                                                                                                                          |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hfus          | 19.93   | kJ/mol | Joback Method      |
| hvap          | 59.31   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 8.50    | eV     | Cheméo Relay (1.0) |
| logp          | 0.113   |        | Crippen Method     |
| mcvol         | 109.490 | ml/mol | McGowan Method     |
| tf            | 341.82  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 261.20 | J/mol×K | 497.48          | Joback Method |
| cpg           | 278.66 | J/mol×K | 538.68          | Joback Method |
| cpg           | 294.68 | J/mol×K | 579.88          | Joback Method |
| cpg           | 309.45 | J/mol×K | 621.08          | Joback Method |
| cpg           | 323.15 | J/mol×K | 662.28          | Joback Method |
| cpg           | 335.96 | J/mol×K | 703.48          | Joback Method |
| cpg           | 348.05 | J/mol×K | 744.68          | Joback Method |

# Pressure Dependent Properties

| Property code | Value  | Unit | Pressure [kPa] | Source       |
|---------------|--------|------|----------------|--------------|
| tbrp          | 382.20 | K    | 3.50           | NIST Webbook |

## Sources

|                           |                                                                                                                                           |
|---------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C177117&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C177117&amp;Units=SI</a> |
| Joback Method:            | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| McGowan Method:           | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| Crippen Method:           | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| Crippen Method:           | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Cheméo Relay (1.0):       |                                                                                                                                           |
| Cheméo Relay (1.0, beta): |                                                                                                                                           |

## Legend

|               |                                                 |
|---------------|-------------------------------------------------|
| <b>cpg:</b>   | Ideal gas heat capacity                         |
| <b>hfus:</b>  | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>  | Enthalpy of vaporization at standard conditions |
| <b>ie:</b>    | Ionization energy                               |
| <b>logp:</b>  | Octanol/Water partition coefficient             |
| <b>mcvol:</b> | McGowan's characteristic volume                 |
| <b>tbrp:</b>  | Boiling point at reduced pressure               |
| <b>tf:</b>    | Normal melting (fusion) point                   |

Latest version available from:

<https://www.chemeo.com/cid/27-441-2/1-4-Dioxa-8-azaspiro-4-5-decane.pdf>

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