# Pyrithyldione

| | |
|---|---|
| **Other names:** | 2,4(1H,3H)-Pyridinedione, 3,3-diethyl- |
| | Benedorm |
| | Didropyridine |
| | Dihydroprylone |
| | Nu 903 |
| | Persedon |
| | Persidon |
| | Presidon |
| | Prezidon |
| | Pyridion |
| | Pyridione |
| | Pyrithyldion |
| | Tetridin |
| | Tetridine |
| | 3,3-Diethyl-2,4(1H,3H)-pyridinedione |
| | 3,3-Diethyl-2,4-dioxotetrahydropyridine |
| | 3,3-Diethylpyridine-2,4(1H,3H)-dione |
| | 3,3-Diethyl-2,4-pyridinedione |
| | 2,4-Dioxo-3,3-diethyltetrahydropyridine |
| | 3,3-Diethyl-1H-pyridine-2,4-dione |
| | NSC 89733 |
| **Inchi:** | InChI=1S/C9H13NO2/c1-3-9(4-2)7(11)5-6-10-8(9)12/h5-6H,3-4H2,1-2H3,(H,10,12) |
| **InchiKey:** | NZASCBIBXNPDMH-UHFFFAOYSA-N |
| **Formula:** | C9H13NO2 |
| **SMILES:** | CCC1(CC)C(=O)C=CNC1=O |
| **Mol. weight [g/mol]:** | 167.21 |
| **CAS:** | 77-04-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -83.65 | kJ/mol | Joback Method |
| hf | -339.34 | kJ/mol | Joback Method |
| hfus | 14.44 | kJ/mol | Joback Method |
| hvap | 50.45 | kJ/mol | Joback Method |
| log10ws | -1.84 | | Crippen Method |
| logp | 1.005 | | Crippen Method |

| | | | |
|---|---|---|---|
| mcvol | 135.630 | ml/mol | McGowan Method |
| pc | 3456.14 | kPa | Joback Method |
| rinpol | 1520.00 | | NIST Webbook |
| rinpol | 1530.00 | | NIST Webbook |
| rinpol | 1510.00 | | NIST Webbook |
| rinpol | 1557.00 | | NIST Webbook |
| rinpol | 1520.00 | | NIST Webbook |
| tb | 608.46 | K | Joback Method |
| tc | 856.42 | K | Joback Method |
| tf | 464.70 | K | Joback Method |
| vc | 0.507 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 345.82 | J/mol×K | 608.46 | Joback Method |
| cpg | 362.01 | J/mol×K | 649.79 | Joback Method |
| cpg | 377.42 | J/mol×K | 691.11 | Joback Method |
| cpg | 392.12 | J/mol×K | 732.44 | Joback Method |
| cpg | 406.16 | J/mol×K | 773.77 | Joback Method |
| cpg | 419.61 | J/mol×K | 815.10 | Joback Method |
| cpg | 432.53 | J/mol×K | 856.42 | Joback Method |

# Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---|---|---|---|---|
| tbrp | 461.20 | K | 1.90 | NIST Webbook |

# Sources

**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=C77043&Units=SI

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |
| **tbrp:** | Boiling point at reduced pressure |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |