# 4-O-Acetyl-2,5-di-O-methyl-3,6-dideoxy-d-gluconit

**Other names:** 4-O-Acetyl-2,5-di-O-methyl-3,6-dideoxygluconitrile
**Inchi:** InChI=1S/C10H17NO4/c1-7(13-3)10(15-8(2)12)5-9(6-11)14-4/h7,9-10H,5H2,1-4H3
**InchiKey:** UIOZESJFWPMERW-UHFFFAOYSA-N
**Formula:** C10H17NO4
**SMILES:** COC(C#N)CC(OC(C)=O)C(C)OC
**Mol. weight [g/mol]:** 215.25

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -284.74 | kJ/mol | Joback Method |
| hf | -609.93 | kJ/mol | Joback Method |
| hfus | 17.76 | kJ/mol | Joback Method |
| hvap | 61.14 | kJ/mol | Joback Method |
| log10ws | -1.25 | | Crippen Method |
| logp | 0.882 | | Crippen Method |
| mcvol | 172.320 | ml/mol | McGowan Method |
| pc | 2129.52 | kPa | Joback Method |
| ripol | 1335.00 | | NIST Webbook |
| ripol | 1335.00 | | NIST Webbook |
| tb | 650.09 | K | Joback Method |
| tc | 846.02 | K | Joback Method |
| tf | 339.07 | K | Joback Method |
| vc | 0.663 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 455.04 | J/mol×K | 650.09 | Joback Method |
| cpg | 467.93 | J/mol×K | 682.75 | Joback Method |
| cpg | 480.19 | J/mol×K | 715.40 | Joback Method |
| cpg | 491.80 | J/mol×K | 748.06 | Joback Method |
| cpg | 502.74 | J/mol×K | 780.71 | Joback Method |
| cpg | 513.01 | J/mol×K | 813.37 | Joback Method |
| cpg | 522.58 | J/mol×K | 846.02 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U101803&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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

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|---|---|
| **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 |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |