# 2-Furylglyoxylonitrile

**Other names:** 2-Furanacetonitrile, «alpha»-oxo-
2-Furanglyoxylonitrile
2-furoyl cyanide
**Inchi:** InChI=1S/C6H3NO2/c7-4-5(8)6-2-1-3-9-6/h1-3H
**InchiKey:** BITJKGFKDMCINV-UHFFFAOYSA-N
**Formula:** C6H3NO2
**SMILES:** N#CC(=O)c1ccco1
**Mol. weight [g/mol]:** 121.09

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -11.97 | kJ/mol | Cheméo Relay (1.0) |
| hvap | 55.12 | kJ/mol | Cheméo Relay (1.0) |
| ie | 9.90 | eV | Cheméo Relay (1.0) |
| log10ws | -0.85 | | Cheméo Relay (1.0) |
| logp | 0.986 | | Crippen Method |
| mcvol | 84.760 | ml/mol | McGowan Method |
| tb | 443.53 | K | Cheméo Relay (1.0) |
| tf | 356.43 | K | Cheméo Relay (1.0) |

# Sources

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**Cheméo Relay (1.0):**
**Cheméo Relay (1.0, beta):**
**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=C6047912&Units=SI
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# Legend

| | |
|---|---|
| **hf:** | Enthalpy of formation at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |