# 2-(3-Hydroxyphenyl)acetonitrile

**Inchi:** InChI=1S/C8H7NO/c9-5-4-7-2-1-3-8(10)6-7/h1-3,6,10H,4H2
**InchiKey:** IEOUEWOHAFNQCO-UHFFFAOYSA-N
**Formula:** C8H7NO
**SMILES:** N#CCc1cccc(O)c1
**Mol. weight [g/mol]:** 133.15
**CAS:** 25263-44-9

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 107.45 | kJ/mol | Joback Method |
| hf | 15.65 | kJ/mol | Joback Method |
| hfus | 17.81 | kJ/mol | Joback Method |
| hvap | 59.17 | kJ/mol | Joback Method |
| log10ws | -1.69 | | Crippen Method |
| logp | 1.458 | | Crippen Method |
| mcvol | 107.070 | ml/mol | McGowan Method |
| pc | 4266.28 | kPa | Joback Method |
| rinpol | 1493.90 | | NIST Webbook |
| rinpol | 1493.90 | | NIST Webbook |
| tb | 591.82 | K | Joback Method |
| tc | 834.93 | K | Joback Method |
| tf | 383.05 | K | Joback Method |
| vc | 0.367 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 243.07 | J/mol×K | 591.82 | Joback Method |
| cpg | 252.07 | J/mol×K | 632.34 | Joback Method |
| cpg | 260.36 | J/mol×K | 672.86 | Joback Method |
| cpg | 268.02 | J/mol×K | 713.37 | Joback Method |
| cpg | 275.14 | J/mol×K | 753.89 | Joback Method |
| cpg | 281.83 | J/mol×K | 794.41 | Joback Method |
| cpg | 288.17 | J/mol×K | 834.93 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C25263449&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |