# Benzonitrile, 2,4,6-trimethyl-

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|---|---|
| **Other names:** | 2,4,6-Trimethylbenzonitrile |
| | Cyanomesitylene |
| | Mesitonitrile |
| | Mesitylnitrile |
| | «beta»-Isodurylonitrile |
| | Â«betaÂ»-Isodurylonitrile |
| **Inchi:** | InChI=1S/C10H11N/c1-7-4-8(2)10(6-11)9(3)5-7/h4-5H,1-3H3 |
| **InchiKey:** | SNIZBGQMWRHNDY-UHFFFAOYSA-N |
| **Formula:** | C10H11N |
| **SMILES:** | Cc1cc(C)c(C#N)c(C)c1 |
| **Mol. weight [g/mol]:** | 145.20 |
| **CAS:** | 2571-52-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -5513.60 ± 2.80 | kJ/mol | NIST Webbook |
| chs | -5530.70 ± 0.90 | kJ/mol | NIST Webbook |
| gf | 250.02 | kJ/mol | Joback Method |
| hf | 106.40 ± 2.30 | kJ/mol | NIST Webbook |
| hf | 84.50 ± 3.00 | kJ/mol | NIST Webbook |
| hfs | 23.50 ± 1.60 | kJ/mol | NIST Webbook |
| hfs | 6.50 ± 2.80 | kJ/mol | NIST Webbook |
| hfus | 15.50 | kJ/mol | Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study |
| hsub | 78.00 | kJ/mol | NIST Webbook |
| hsub | 82.90 ± 1.60 | kJ/mol | NIST Webbook |
| hsub | 82.90 | kJ/mol | NIST Webbook |
| hsub | 82.90 ± 1.60 | kJ/mol | NIST Webbook |
| hsub | 78.00 ± 1.20 | kJ/mol | NIST Webbook |
| hvap | 52.59 | kJ/mol | Joback Method |
| log10ws | -3.25 | | Crippen Method |
| logp | 2.484 | | Crippen Method |
| mcvol | 129.380 | ml/mol | McGowan Method |
| pc | 2721.17 | kPa | Joback Method |
| tb | 571.90 | K | Joback Method |

| | | | |
|---|---|---|---|
| tc | 798.39 | K | Joback Method |
| tf | 331.43 | K | Joback Method |
| vc | 0.513 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 286.16 | J/mol×K | 571.90 | Joback Method |
| cpg | 297.82 | J/mol×K | 609.65 | Joback Method |
| cpg | 308.84 | J/mol×K | 647.40 | Joback Method |
| cpg | 319.24 | J/mol×K | 685.14 | Joback Method |
| cpg | 329.03 | J/mol×K | 722.89 | Joback Method |
| cpg | 338.24 | J/mol×K | 760.64 | Joback Method |
| cpg | 346.88 | J/mol×K | 798.39 | Joback Method |
| cps | 220.50 | J/mol×K | 298.15 | NIST Webbook |

# Correlations

| Information | Value |
|---|---|
| Property code | pvap |
| Equation | ln(Pvp) = A + B/(T + C) |
| Coeff. A | 1.52324e+01 |
| Coeff. B | -4.63378e+03 |
| Coeff. C | -9.09130e+01 |
| Temperature range (K), min. | 400.97 |
| Temperature range (K), max. | 557.98 |

# Sources

| | |
|---|---|
| **Benchmark thermochemistry of methylbenzonitriles: Experimental and theoretical study:** | https://www.doi.org/10.1016/j.jct.2015.07.025 |
| **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=C2571520&Units=SI |
| **The Yaws Handbook of Vapor Pressure:** | https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **cps:** | Solid phase heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hsub:** | Enthalpy of sublimation 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 |
| **pvap:** | Vapor pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |