

# 2,4,6-Trimethoxybenzonitrile

|                      |  |  |  |
|----------------------|--|--|--|
| Other names:         | Benzonitrile, 2,4,6-trimethoxy-                                    |  |  |
| Inchi:               | InChI=1S/C10H11NO3/c1-12-7-4-9(13-2)8(6-11)10(5-7)14-3/h4-5H,1-3H3 |  |  |
| InchiKey:            | GBRHJUMDNWL SCT-UHFFFAOYSA-N                                       |  |  |
| Formula:             | C10H11NO3  |  |  |
| SMILES:              | COc1cc(OC)c(C#N)c(OC)c1  |  |  |
| Mol. weight [g/mol]: | 193.20   |  |  |
| CAS:                 | 2571-54-2  |  |  |

## Physical Properties

| Property code | Value           | Unit    | Source         |
|---------------|-----------------|---------|----------------|
| chs           | -5150.00 ± 0.90 | kJ/mol  | NIST Webbook   |
| gf            | -64.98          | kJ/mol  | Joback Method  |
| hf            | -244.60 ± 2.60  | kJ/mol  | NIST Webbook   |
| hfs           | -357.20 ± 1.60  | kJ/mol  | NIST Webbook   |
| hfus          | 19.60           | kJ/mol  | Joback Method  |
| hsub          | 112.60 ± 2.00   | kJ/mol  | NIST Webbook   |
| hsub          | 112.60 ± 2.00   | kJ/mol  | NIST Webbook   |
| hvap          | 59.82           | kJ/mol  | Joback Method  |
| log10ws       | -2.18           |         | Crippen Method |
| logp          | 1.584           |         | Crippen Method |
| mcvol         | 146.990         | ml/mol  | McGowan Method |
| pc            | 2581.96         | kPa     | Joback Method  |
| tb            | 639.16          | K       | Joback Method  |
| tc            | 857.09          | K       | Joback Method  |
| tf            | 398.12          | K       | Joback Method  |
| vc            | 0.568           | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 354.92 | J/mol×K | 639.16          | Joback Method |
| cpg           | 366.33 | J/mol×K | 675.48          | Joback Method |
| cpg           | 377.19 | J/mol×K | 711.80          | Joback Method |
| cpg           | 387.45 | J/mol×K | 748.13          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 397.08 | J/mol×K | 784.45 | Joback Method |
| cpg | 406.05 | J/mol×K | 820.77 | Joback Method |
| cpg | 414.33 | J/mol×K | 857.09 | Joback Method |

## Sources

|                 |   |
|-----------------|---|
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                       |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2571542&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2571542&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |

## Legend

|                 |  |
|-----------------|--|
| <b>chs:</b>     | Standard solid enthalpy of combustion                    |
| <b>cpg:</b>     | Ideal gas heat capacity                                  |
| <b>gf:</b>      | Standard Gibbs free energy of formation                  |
| <b>hf:</b>      | Enthalpy of formation at standard conditions             |
| <b>hfs:</b>     | Solid phase enthalpy of formation at standard conditions |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions                |
| <b>hsub:</b>    | Enthalpy of sublimation at standard conditions           |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions          |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l                       |
| <b>logp:</b>    | Octanol/Water partition coefficient                      |
| <b>mcvol:</b>   | McGowan's characteristic volume                          |
| <b>pc:</b>      | Critical Pressure  |
| <b>tb:</b>      | Normal Boiling Point Temperature                         |
| <b>tc:</b>      | Critical Temperature                                     |
| <b>tf:</b>      | Normal melting (fusion) point                            |
| <b>vc:</b>      | Critical Volume  |

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