

# 2-(phenylhydrazinylidene)propanedinitrile

**Inchi:** InChI=1S/C9H6N4/c10-6-9(7-11)13-12-8-4-2-1-3-5-8/h1-5,12H  
**InchiKey:** MENUYOGJXCXAFU-UHFFFAOYSA-N  
**Formula:** C9H6N4  
**SMILES:** N#CC(C#N)=NNc1ccccc1  
**Mol. weight [g/mol]:** 170.18

## Physical Properties

| Property code | Value   | Unit   | Source                               |
|---------------|---------|--------|--------------------------------------|
| hf            | 463.10  | kJ/mol | Joback Method                        |
| hvap          | 68.69   | kJ/mol | Joback Method                        |
| log10ws       | -0.36   |        | Aqueous Solubility Prediction Method |
| logp          | 1.502   |        | Crippen Method                       |
| mcvol         | 132.330 | ml/mol | McGowan Method                       |
| pc            | 2805.41 | kPa    | Joback Method                        |
| tb            | 762.89  | K      | Joback Method                        |
| tc            | 1019.19 | K      | Joback Method                        |

## Sources

**Aqueous Solubility Prediction Method:** <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

**hf:** Enthalpy of formation 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  
**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature

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