

# 2-Fluorobenzhydrazide

|                      |                                                                  |
|----------------------|------------------------------------------------------------------|
| Inchi:               | InChI=1S/C7H7FN2O/c8-6-4-2-1-3-5(6)7(11)10-9/h1-4H,9H2,(H,10,11) |
| InchiKey:            | YJCCKQQVXNNAAR-UHFFFAOYSA-N                                      |
| Formula:             | C7H7FN2O                                                         |
| SMILES:              | NNC(=O)c1ccccc1F                                                 |
| Mol. weight [g/mol]: | 154.14                                                           |
| CAS:                 | 446-24-2                                                         |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -57.05  | kJ/mol  | Joback Method  |
| hf            | -184.18 | kJ/mol  | Joback Method  |
| hfus          | 22.51   | kJ/mol  | Joback Method  |
| hvap          | 57.12   | kJ/mol  | Joback Method  |
| log10ws       | -2.15   |         | Crippen Method |
| logp          | 0.429   |         | Crippen Method |
| mcvol         | 109.030 | ml/mol  | McGowan Method |
| pc            | 4528.58 | kPa     | Joback Method  |
| tb            | 567.06  | K       | Joback Method  |
| tc            | 792.48  | K       | Joback Method  |
| tf            | 394.03  | K       | Joback Method  |
| vc            | 0.407   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 249.98 | J/mol×K | 567.06          | Joback Method |
| cpg           | 259.91 | J/mol×K | 604.63          | Joback Method |
| cpg           | 269.15 | J/mol×K | 642.20          | Joback Method |
| cpg           | 277.72 | J/mol×K | 679.77          | Joback Method |
| cpg           | 285.65 | J/mol×K | 717.34          | Joback Method |
| cpg           | 292.98 | J/mol×K | 754.91          | Joback Method |
| cpg           | 299.72 | J/mol×K | 792.48          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C446242&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C446242&amp;Units=SI</a> |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <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>hfus:</b>    | Enthalpy of fusion 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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