

# Benzo[f]quinoline

|                      |                                                                                                                                                |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1-Azaphenanthrene<br>5,6-Benzo[f]quinoline<br>5,6-Benzoquinoline<br>b-Naphthoquinoline<br>«beta»-Naphthoquinoline<br>Â«betaÂ»-Naphthoquinoline |
| Inchi:               | InChI=1S/C13H9N/c1-2-5-11-10(4-1)7-8-13-12(11)6-3-9-14-13/h1-9H                                                                                |
| InchiKey:            | HCAUQPZEWLULFJ-UHFFFAOYSA-N                                                                                                                    |
| Formula:             | C13H9N                                                                                                                                         |
| SMILES:              | c1ccc2c(c1)ccc1ncccc12                                                                                                                         |
| Mol. weight [g/mol]: | 179.22                                                                                                                                         |
| CAS:                 | 85-02-9                                                                                                                                        |

## Physical Properties

| Property code | Value           | Unit   | Source                               |
|---------------|-----------------|--------|--------------------------------------|
| chs           | -6552.50 ± 6.20 | kJ/mol | NIST Webbook                         |
| hf            | 233.70 ± 7.40   | kJ/mol | NIST Webbook                         |
| hsub          | 83.10 ± 6.20    | kJ/mol | NIST Webbook                         |
| ie            | 8.14            | eV     | NIST Webbook                         |
| ie            | 8.40 ± 0.10     | eV     | NIST Webbook                         |
| ie            | 8.14 ± 0.02     | eV     | NIST Webbook                         |
| log10ws       | -3.36           |        | Aqueous Solubility Prediction Method |
| logp          | 3.388           |        | Crippen Method                       |
| mcvol         | 141.330         | ml/mol | McGowan Method                       |
| rinpol        | 1807.00         |        | NIST Webbook                         |
| rinpol        | 1840.00         |        | NIST Webbook                         |
| rinpol        | 1800.00         |        | NIST Webbook                         |
| rinpol        | 306.86          |        | NIST Webbook                         |
| rinpol        | 306.86          |        | NIST Webbook                         |
| rinpol        | 307.30          |        | NIST Webbook                         |
| rinpol        | 308.27          |        | NIST Webbook                         |
| rinpol        | 306.96          |        | NIST Webbook                         |
| rinpol        | 307.30          |        | NIST Webbook                         |
| rinpol        | 307.94          |        | NIST Webbook                         |
| rinpol        | 309.25          |        | NIST Webbook                         |
| rinpol        | 307.94          |        | NIST Webbook                         |

|        |               |   |              |
|--------|---------------|---|--------------|
| rinpol | 1840.00       |   | NIST Webbook |
| rinpol | 307.94        |   | NIST Webbook |
| tf     | 367.00        | K | NIST Webbook |
| tf     | 364.80 ± 2.00 | K | NIST Webbook |

## Temperature Dependent Properties

| Property code | Value        | Unit   | Temperature [K] | Source       |
|---------------|--------------|--------|-----------------|--------------|
| hsubt         | 83.10 ± 3.60 | kJ/mol | 305.50          | NIST Webbook |

## Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 623.20        | K    | 96.10          | NIST Webbook |
| tbrp          | 623.00        | K    | 96.10          | NIST Webbook |
| tbrp          | 485.50 ± 2.50 | K    | 2.90           | NIST Webbook |

## Sources

|                                       |                                                                                                                                                                                               |
|---------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 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=C85029&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C85029&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>                                                                                     |
| Aqueous Solubility Prediction Method: | <a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a> |

## Legend

|          |                                                |
|----------|------------------------------------------------|
| chs:     | Standard solid enthalpy of combustion          |
| hf:      | Enthalpy of formation at standard conditions   |
| hsub:    | Enthalpy of sublimation at standard conditions |
| hsubt:   | Enthalpy of sublimation at a given temperature |
| ie:      | Ionization energy                              |
| log10ws: | Log10 of Water solubility in mol/l             |

|                |                                     |
|----------------|-------------------------------------|
| <b>logp:</b>   | Octanol/Water partition coefficient |
| <b>mcvol:</b>  | McGowan's characteristic volume     |
| <b>rinpol:</b> | Non-polar retention indices         |
| <b>tbrp:</b>   | Boiling point at reduced pressure   |
| <b>tf:</b>     | Normal melting (fusion) point       |

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