

5-nitroindole

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| Other names: | indole, 5-nitro- |
| Inchi: | InChI=1S/C8H6N2O2/c11-10(12)7-1-2-8-6(5-7)3-4-9-8/h1-5,9H |
| InchiKey: | OZFPSOBLQZPIAV-UHFFFAOYSA-N |
| Formula: | C8H6N2O2 |
| SMILES: | O=[N+](O-)[c1ccc2[nH]ccc2c1] |
| Mol. weight [g/mol]: | 162.15 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.15 | | Crippen Method |
| logp | 1.594 | | Crippen Method |
| mcvol | 112.060 | ml/mol | McGowan Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|----------|------|-----------------|--|
| psub | 9.42e-05 | kPa | 353.15 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 9.30e-05 | kPa | 353.15 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 9.30e-05 | kPa | 353.15 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 1.15e-04 | kPa | 355.20 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |

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| psub | 1.12e-04 | kPa | 355.20 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 1.37e-04 | kPa | 357.18 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 1.34e-04 | kPa | 357.18 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 1.31e-04 | kPa | 357.18 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 1.72e-04 | kPa | 359.15 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 1.70e-04 | kPa | 359.15 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 1.67e-04 | kPa | 359.15 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 2.00e-04 | kPa | 361.19 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 2.01e-04 | kPa | 361.19 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 2.44e-04 | kPa | 363.17 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |

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| psub | 2.36e-04 | kPa | 363.17 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 3.14e-04 | kPa | 365.16 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 3.04e-04 | kPa | 365.16 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 2.93e-04 | kPa | 365.16 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 3.80e-04 | kPa | 367.19 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 3.69e-04 | kPa | 367.19 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 3.54e-04 | kPa | 367.19 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 4.45e-04 | kPa | 369.17 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 4.39e-04 | kPa | 369.17 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 4.32e-04 | kPa | 369.17 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |

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| psub | 5.52e-04 | kPa | 371.17 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 5.46e-04 | kPa | 371.17 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 5.33e-04 | kPa | 371.17 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 6.82e-04 | kPa | 373.19 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 6.53e-04 | kPa | 373.19 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 6.31e-04 | kPa | 373.19 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 8.01e-04 | kPa | 375.17 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |
| psub | 7.69e-04 | kPa | 375.17 | Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline |

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Experimental study on the thermochemistry of 5-nitroindole and 5-nitroindoline

<https://www.doi.org/10.1016/j.jct.2008.09.014>

McGowan Method:

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

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| psub: | Sublimation pressure |

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