# 1H-Pyrrole-2-carboxaldehyde

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|---|---|
| **Other names:** | Pyrrole-2-carboxaldehyde |
| | Pyrrole-2-aldehyde |
| | 2-Formylpyrrole |
| | 2-Pyrrolylcarboxaldehyde |
| | «alpha»-Pyrrolaldehyde |
| | 2-Pyrrolecarbaldehyde |
| | 2-Pyrrolecarboxaldehyde |
| | 1H-Pyrrole-2-carboxyaldehyde |
| | 2-Carboxaldehyde-1H-pyrrole |
| | 2-Pyrrolaldehyde |
| | 2-Pyrrolcarbaldehyde |
| | NSC 112885 |
| | NSC 66394 |
| | 1-Pyrrole-2-carboxaldehyde |
| | 1( H)-pyrrole carboxaldehyde |
| | Pyrrol-2-carboxaldehyde |
| | pyrrole-2-carbaldehyde |
| **Inchi:** | InChI=1S/C5H5NO/c7-4-5-2-1-3-6-5/h1-4,6H |
| **InchiKey:** | ZSKGQVFRTSEPJT-UHFFFAOYSA-N |
| **Formula:** | C5H5NO |
| **SMILES:** | O=Cc1ccc[nH]1 |
| **Mol. weight [g/mol]:** | 95.10 |
| **CAS:** | 1003-29-8 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -2575.70 ± 2.50 | kJ/mol | NIST Webbook |
| hfs | -106.40 ± 2.50 | kJ/mol | NIST Webbook |
| ie | 8.93 ± 0.05 | eV | NIST Webbook |
| log10ws | -0.93 | | Crippen Method |
| logp | 0.345 | | Crippen Method |
| mcvol | 73.400 | ml/mol | McGowan Method |
| rinpol | 1031.00 | | NIST Webbook |
| rinpol | 971.00 | | NIST Webbook |
| rinpol | 1008.00 | | NIST Webbook |
| rinpol | 1047.00 | | NIST Webbook |
| rinpol | 1013.00 | | NIST Webbook |

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|---|---|---|
| rinpol | 983.00 | NIST Webbook |
| rinpol | 1013.00 | NIST Webbook |
| rinpol | 989.00 | NIST Webbook |
| rinpol | 1008.00 | NIST Webbook |
| rinpol | 1018.00 | NIST Webbook |
| rinpol | 1030.00 | NIST Webbook |
| rinpol | 1030.00 | NIST Webbook |
| rinpol | 1012.00 | NIST Webbook |
| rinpol | 988.00 | NIST Webbook |
| rinpol | 1009.00 | NIST Webbook |
| rinpol | 1043.00 | NIST Webbook |
| rinpol | 1016.00 | NIST Webbook |
| rinpol | 1005.00 | NIST Webbook |
| rinpol | 986.00 | NIST Webbook |
| rinpol | 1015.00 | NIST Webbook |
| rinpol | 1009.00 | NIST Webbook |
| rinpol | 1030.00 | NIST Webbook |
| rinpol | 1015.00 | NIST Webbook |
| rinpol | 1009.00 | NIST Webbook |
| rinpol | 997.00 | NIST Webbook |
| ripol | 2028.00 | NIST Webbook |
| ripol | 2032.00 | NIST Webbook |
| ripol | 2032.00 | NIST Webbook |
| ripol | 2030.00 | NIST Webbook |
| ripol | 2030.00 | NIST Webbook |
| ripol | 2044.00 | NIST Webbook |
| ripol | 2067.00 | NIST Webbook |
| ripol | 2059.00 | NIST Webbook |
| ripol | 2010.00 | NIST Webbook |
| ripol | 2035.00 | NIST Webbook |
| ripol | 2023.00 | NIST Webbook |
| ripol | 2044.00 | NIST Webbook |
| ripol | 2036.00 | NIST Webbook |
| ripol | 2067.00 | NIST Webbook |
| ripol | 2009.00 | NIST Webbook |
| ripol | 2006.00 | NIST Webbook |
| ripol | 1978.00 | NIST Webbook |
| ripol | 2032.00 | NIST Webbook |
| ripol | 2038.00 | NIST Webbook |
| ripol | 2044.00 | NIST Webbook |
| ripol | 1990.00 | NIST Webbook |
| ripol | 2048.00 | NIST Webbook |
| ripol | 2019.00 | NIST Webbook |
| ripol | 1997.00 | NIST Webbook |

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|---|---|---|---|
| ripol | 2039.00 | | NIST Webbook |
| ripol | 1976.00 | | NIST Webbook |
| ripol | 2044.00 | | NIST Webbook |
| ripol | 2013.00 | | NIST Webbook |
| tb | 491.20 | K | NIST Webbook |

# Sources

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|---|---|
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1003298&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **ripol:** | Polar retention indices |
| **tb:** | Normal Boiling Point Temperature |