

1H-Pyrrole, 3-ethyl-2,4-dimethyl-

| | |
|-----------------------------|--|
| Other names: | 2,4-Dimethyl-3-ethylpyrrole 3-Ethyl-2,4-dimethyl-1H-pyrrole 3-Ethyl-2,4-dimethylpyrrole Cryptopyrrole Kryptopyrrol Kryptopyrrole NSC 62025 Pyrrole, 3-ethyl-2,4-dimethyl- |
| Inchi: | InChI=1S/C8H13N/c1-4-8-6(2)5-9-7(8)3/h5,9H,4H2,1-3H3 |
| InchiKey: | ZEBBLOXDLGIMEG-UHFFFAOYSA-N |
| Formula: | C8H13N |
| SMILES: | CCc1c(C)c[nH]c1C |
| Mol. weight [g/mol]: | 123.20 |
| CAS: | 517-22-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------------|--------|----------------|
| log10ws | -2.44 | | Crippen Method |
| logp | 1.712 | | Crippen Method |
| mcvol | 114.100 | ml/mol | McGowan Method |
| rinpol | 988.00 | | NIST Webbook |
| rinpol | 988.00 | | NIST Webbook |
| tb | 470.50 ± 0.40 | K | NIST Webbook |
| tb | 470.45 ± 0.40 | K | NIST Webbook |
| tf | 286.75 ± 0.20 | K | NIST Webbook |
| tf | 286.80 ± 0.30 | K | NIST Webbook |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 470.20 | K | 94.70 | NIST Webbook |
| tbrp | 369.20 | K | 2.10 | NIST Webbook |

Correlations

| Information | Value |
|-----------------------------|-------------------------------|
| Property code | pvap |
| Equation | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A | 1.52474e+01 |
| Coeff. B | -4.23081e+03 |
| Coeff. C | -7.24080e+01 |
| Temperature range (K), min. | 336.90 |
| Temperature range (K), max. | 498.22 |

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C517226&Units=SI>

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcbvol: | McGowan's characteristic volume |
| pvap: | Vapor pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tbrp: | Boiling point at reduced pressure |
| tf: | Normal melting (fusion) point |

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