

# 4-Ethyl-3,5-dimethyl-1H-pyrrole-2-carboxaldehyde

|                      |                                                                                                        |
|----------------------|--------------------------------------------------------------------------------------------------------|
| Other names:         | 1H-Pyrrole-2-carboxaldehyde, 4-ethyl-3,5-dimethyl-<br>1H-Pyrrole-2-carbaldehyde, 4-ethyl-3,5-dimethyl- |
| Inchi:               | InChI=1S/C9H13NO/c1-4-8-6(2)9(5-11)10-7(8)3/h5,10H,4H2,1-3H3                                           |
| InchiKey:            | VHIKIUXLJPZNCA-UHFFFAOYSA-N                                                                            |
| Formula:             | C9H13NO                                                                                                |
| SMILES:              | CCc1c(C)[nH]c(C=O)c1C                                                                                  |
| Mol. weight [g/mol]: | 151.21                                                                                                 |
| CAS:                 | 6250-80-2                                                                                              |

## Physical Properties

| Property code | Value           | Unit   | Source         |
|---------------|-----------------|--------|----------------|
| chs           | -5144.60 ± 5.00 | kJ/mol | NIST Webbook   |
| hfs           | -254.80 ± 5.00  | kJ/mol | NIST Webbook   |
| log10ws       | -2.69           |        | Crippen Method |
| logp          | 1.525           |        | Crippen Method |
| mcvol         | 129.760         | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6250802&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6250802&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>                                   |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

|          |                                                          |
|----------|----------------------------------------------------------|
| chs:     | Standard solid enthalpy of combustion                    |
| hfs:     | Solid phase enthalpy of formation at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l                       |
| logp:    | Octanol/Water partition coefficient                      |
| mcvol:   | McGowan's characteristic volume                          |

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