

# 5-Chloro-1-ethyl-2-methylbenzimidazole

|                      |                                                                         |
|----------------------|-------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C10H11ClN2/c1-3-13-7(2)12-9-6-8(11)4-5-10(9)13/h4-6H,3H2,1-2H3 |
| InchiKey:            | WOUUWYXDNDKIGX-UHFFFAOYSA-N                                             |
| Formula:             | C10H11ClN2                                                              |
| SMILES:              | CCn1c(C)nc2cc(Cl)ccc21                                                  |
| Mol. weight [g/mol]: | 194.66                                                                  |
| CAS:                 | 2818-76-0                                                               |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.46   |        | Crippen Method |
| logp          | 3.018   |        | Crippen Method |
| mcvol         | 145.040 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| 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>                       |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2818760&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2818760&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>                                   |

## Legend

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

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