

# 1H-benzotriazole, 4,6-difluoro-

|                             |                                                                  |
|-----------------------------|------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C6H3F2N3/c7-3-1-4(8)6-5(2-3)9-11-10-6/h1-2H,(H,9,10,11) |
| <b>InchiKey:</b>            | WWDQELZQQFCUOG-UHFFFAOYSA-N                                      |
| <b>Formula:</b>             | C6H3F2N3                                                         |
| <b>SMILES:</b>              | Fc1cc(F)c2nn[nH]c2c1                                             |
| <b>Mol. weight [g/mol]:</b> | 155.10                                                           |
| <b>CAS:</b>                 | 2208-25-5                                                        |

## Physical Properties

| Property code | Value  | Unit   | Source         |
|---------------|--------|--------|----------------|
| log10ws       | -2.69  |        | Crippen Method |
| logp          | 0.754  |        | Crippen Method |
| mcvol         | 89.960 | ml/mol | McGowan Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C2208255&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2208255&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |

## Legend

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

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