

Oxazole, 4-ethyl-5-methyl

Inchi: InChI=1S/C6H9NO/c1-3-6-5(2)8-4-7-6/h4H,3H2,1-2H3
InchiKey: CRARVVVEJLFERY-UHFFFAOYSA-N
Formula: C6H9NO
SMILES: CCc1ncoc1C
Mol. weight [g/mol]: 111.14

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -6.25 | | Crippen Method |
| logp | 1.545 | | Crippen Method |
| mcvol | 91.790 | ml/mol | McGowan Method |
| ripol | 855.00 | | NIST Webbook |
| ripol | 1201.00 | | NIST Webbook |
| ripol | 1201.00 | | NIST Webbook |
| ripol | 1200.00 | | NIST Webbook |
| ripol | 1222.00 | | NIST Webbook |
| ripol | 1200.00 | | NIST Webbook |
| ripol | 1200.00 | | NIST Webbook |

Sources

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=R61867&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

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