

2-n-Butyl-4-ethyl-5-methyloxazole

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|-----------------------------|---|
| Other names: | Oxazole, 2-butyl-4-ethyl-5-methyl |
| Inchi: | InChI=1S/C10H17NO/c1-4-6-7-10-11-9(5-2)8(3)12-10/h4-7H2,1-3H3 |
| InchiKey: | PGYVZKVDXNIABS-UHFFFAOYSA-N |
| Formula: | C10H17NO |
| SMILES: | CCCCc1nc(CC)c(C)o1 |
| Mol. weight [g/mol]: | 167.25 |
| CAS: | 84028-03-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.89 | | Crippen Method |
| logp | 2.888 | | Crippen Method |
| mcvol | 148.150 | ml/mol | McGowan Method |
| rinpol | 1159.00 | | NIST Webbook |
| rinpol | 1159.00 | | NIST Webbook |
| ripol | 1441.00 | | NIST Webbook |
| ripol | 1441.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | 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=C84028035&Units=SI |

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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