

Oxazole, 2-ethyl-4-methyl-5-propyl

Other names: 2-ethyl-4-methyl-5-propyloxazole
Inchi: InChI=1S/C9H15NO/c1-4-6-8-7(3)10-9(5-2)11-8/h4-6H2,1-3H3
InchiKey: FDMDJAGBUGUESB-UHFFFAOYSA-N
Formula: C9H15NO
SMILES: CCCc1oc(CC)nc1C
Mol. weight [g/mol]: 153.22

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -7.47 | | Crippen Method |
| logp | 2.498 | | Crippen Method |
| mcvol | 134.060 | ml/mol | McGowan Method |
| rinpol | 1079.00 | | NIST Webbook |
| rinpol | 1079.00 | | NIST Webbook |
| rinpol | 1079.00 | | NIST Webbook |
| rinpol | 1071.00 | | NIST Webbook |
| ripol | 1374.00 | | NIST Webbook |
| ripol | 1374.00 | | NIST Webbook |
| ripol | 1374.00 | | 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=R46146&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

Latest version available from:

<https://www.cheméo.com/cid/55-587-0/Oxazole-2-ethyl-4-methyl-5-propyl.pdf>

Generated by Cheméo on 2024-04-27 03:18:50.33635468 +0000 UTC m=+16477179.256931995.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.