

Pyridine, 3-(4-methylpentyl)

Inchi: InChI=1S/C11H17N/c1-10(2)5-3-6-11-7-4-8-12-9-11/h4,7-10H,3,5-6H2,1-2H3
InchiKey: PURGSRBQHMOSXO-UHFFFAOYSA-N
Formula: C11H17N
SMILES: CC(C)CCCc1cccnc1
Mol. weight [g/mol]: 163.26

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.47 | | Crippen Method |
| logp | 3.060 | | Crippen Method |
| mcvol | 152.070 | ml/mol | McGowan Method |
| rinpol | 1303.00 | | NIST Webbook |
| ripol | 1759.00 | | 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=R70503&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

Latest version available from:

<https://www.chemeo.com/cid/79-791-7/Pyridine-3-4-methylpentyl.pdf>

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