

4-Quinazolone, 2-methyl-3-pentyl

Inchi: InChI=1S/C14H18N2O/c1-3-4-7-10-16-11(2)15-13-9-6-5-8-12(13)14(16)17/h5-6,8-9H,3-4H2
InchiKey: XLDMZWAECSDDTG-UHFFFAOYSA-N
Formula: C14H18N2O
SMILES: CCCCCn1c(C)nc2cccc2c1=O
Mol. weight [g/mol]: 230.31

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -4.46 | | Crippen Method |
| logp | 2.895 | | Crippen Method |
| mcvol | 190.730 | ml/mol | McGowan Method |
| rinsol | 2003.00 | | NIST Webbook |
| rinsol | 2003.00 | | NIST Webbook |
| rinsol | 2003.00 | | 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=R64500&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinsol: Non-polar retention indices

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<https://www.chemeo.com/cid/62-750-0/4-Quinazolone-2-methyl-3-pentyl.pdf>

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