

4-Quinazolone, 2-ethyl-3-pentyl

Inchi: InChI=1S/C15H20N2O/c1-3-5-8-11-17-14(4-2)16-13-10-7-6-9-12(13)15(17)18/h6-7,9-10
InchiKey: QRFKUDDRZZYPPR-UHFFFAOYSA-N
Formula: C15H20N2O
SMILES: CCCCCn1c(CC)nc2ccccc2c1=O
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.78		Crippen Method
logp	3.149		Crippen Method
mcvol	204.820	ml/mol	McGowan Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		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=R64489&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

Latest version available from:

<https://www.chemeo.com/cid/124-471-1/4-Quinazolone-2-ethyl-3-pentyl.pdf>

Generated by Cheméo on 2024-04-29 00:59:54.881559546 +0000 UTC m=+16641643.802136856.
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.