

4-Quinazolone, 3-butyl-2-methyl

Inchi: InChI=1S/C13H16N2O/c1-3-4-9-15-10(2)14-12-8-6-5-7-11(12)13(15)16/h5-8H,3-4,9H2,1
InchiKey: WBYGSYVGRKQFJY-UHFFFAOYSA-N
Formula: C13H16N2O
SMILES: CCCc1c(C)nc2ccccc2c1=O
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	2.505		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
rinpol	1915.00		NIST Webbook
rinpol	1915.00		NIST Webbook
rinpol	1915.00		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=R64564&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

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<https://www.chemeo.com/cid/114-255-2/4-Quinazolone-3-butyl-2-methyl.pdf>

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