

4-Quinazolone, 2-methyl-3-propyl

Inchi: InChI=1S/C14H18N2O/c1-3-7-13-15-12-9-6-5-8-11(12)14(17)16(13)10-4-2/h5-6,8-9H,3-4H2
InchiKey: OVNUJWFZARIOQD-UHFFFAOYSA-N
Formula: C14H18N2O
SMILES: CCCc1nc2ccccc2c(=O)n1CCC
Mol. weight [g/mol]: 230.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	2.759		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
rinpol	1826.00		NIST Webbook
rinpol	1826.00		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=R64514&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/120-810-8/4-Quinazolone-2-methyl-3-propyl.pdf>

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