

4-Quinazolone, 3-butyl

Inchi:	InChI=1S/C12H14N2O/c1-2-3-8-14-9-13-11-7-5-4-6-10(11)12(14)15/h4-7,9H,2-3,8H2,1H
InchiKey:	ZZSCVWJRCJHPA-UHFFFAOYSA-N
Formula:	C12H14N2O
SMILES:	CCCCn1cnc2cccc2c1=O
Mol. weight [g/mol]:	202.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.56		Crippen Method
logp	2.197		Crippen Method
mcvol	162.550	ml/mol	McGowan Method
rinpola	1835.00		NIST Webbook
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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=R64546&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/58-081-8/4-Quinazolone-3-butyl.pdf>

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