4-Quinazolone, 2-butyl-3-methyl

Inchi:	InChI=1S/C13H16N2O/c1-3-4-9-12-14-11-8-6-5-7-10(11)13(16)15(12)2/h5-8H,3-4,9H2,1
InchiKey:	NKMXYZJTOQNVGH-UHFFFAOYSA-N
Formula:	C13H16N2O
SMILES:	CCCCc1nc2ccccc2c(=O)n1C
Mol. weight [g/mol]:	216.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.39		Crippen Method
logp	2.276		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R64461&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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