

4-Quinazolone, 2-butyl

Other names:	Quinazolin-4-one, 2-butyl
Inchi:	InChI=1S/C12H14N2O/c1-2-3-8-11-13-10-7-5-4-6-9(10)12(15)14-11/h4-7H,2-3,8H2,1H3
InchiKey:	WBFIFMJPHUALRV-UHFFFAOYSA-N
Formula:	C12H14N2O
SMILES:	CCCCc1nc2ccccc2c(=O)[nH]1
Mol. weight [g/mol]:	202.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.32		Crippen Method
logp	1.784		Crippen Method
mcvol	162.550	ml/mol	McGowan Method
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook
rinpol	1955.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R64443&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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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