

4-Quinazolone, 3-ethyl-2-methyl

Inchi:	InChI=1S/C11H12N2O/c1-3-13-8(2)12-10-7-5-4-6-9(10)11(13)14/h4-7H,3H2,1-2H3
InchiKey:	UMQKDYHNDQNEBD-UHFFFAOYSA-N
Formula:	C11H12N2O
SMILES:	CCn1c(C)nc2ccccc2c1=O
Mol. weight [g/mol]:	188.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	1.725		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
rinpol	1749.00		NIST Webbook
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rinpol	1749.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R64578&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/91-043-3/4-Quinazolone-3-ethyl-2-methyl.pdf>

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