4-Quinazolone, 2-ethyl-3-methyl

Inchi: InChI=1S/C11H12N2O/c1-3-10-12-9-7-5-4-6-8(9)11(14)13(10)2/h4-7H,3H2,1-2H3
InchiKey: QCKGJLGHIVZYGZ-UHFFFAOYSA-N
Formula: C11H12N2O
SMILES: CCc1nc2ccccc2c(=O)n1C
Mol. weight [g/mol]: 188.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.55		Crippen Method
logp	1.496		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64475&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