4-Quinazolone, 2-propyl

Inchi: InChI=1S/C11H12N2O/c1-2-5-10-12-9-7-4-3-6-8(9)11(14)13-10/h3-4,6-7H,2,5H2,1H3,(H
InchiKey: MFAZKHYKVSPPIB-UHFFFAOYSA-N
Formula: C11H12N2O
SMILES: CCCc1nc2ccccc2c(=O)[nH]1
Mol. weight [g/mol]: 188.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.90		Crippen Method
logp	1.394		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
rinpol	1853.00		NIST Webbook
rinpol	1853.00		NIST Webbook
rinpol	1853.00		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=R64532&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

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