4-Quinazolone, 2-pentyl

Inchi: InChI=1S/C13H16N2O/c1-2-3-4-9-12-14-11-8-6-5-7-10(11)13(16)15-12/h5-8H,2-4,9H2,1
InchiKey: ZFDMQFNZNRCSQN-UHFFFAOYSA-N
Formula: C13H16N2O
SMILES: CCCCCc1nc2ccccc2c(=O)[nH]1
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.74		Crippen Method
logp	2.174		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64528&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