4-Quinazolone, 3-pentyl

Inchi: InChI=1S/C13H16N2O/c1-2-3-6-9-15-10-14-12-8-5-4-7-11(12)13(15)16/h4-5,7-8,10H,2-3
InchiKey: NWGZMFRPINJEAC-UHFFFAOYSA-N
Formula: C13H16N2O
SMILES: CCCCCn1cnc2ccccc2c1=O
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	2.587		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
rinpol	1926.00		NIST Webbook
rinpol	1926.00		NIST Webbook
rinpol	1926.00		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=R64621&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