4-Quinazolone, 2-ethyl-3-pentyl

Inchi: InChI=1S/C15H20N2O/c1-3-5-8-11-17-14(4-2)16-13-10-7-6-9-12(13)15(17)18/h6-7,9-10H
InchiKey: QRFKUDDRZZYPPR-UHFFFAOYSA-N
Formula: C15H20N2O
SMILES: CCCCCn1c(CC)nc2ccccc2c1=O
Mol. weight [g/mol]: 244.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.78		Crippen Method
logp	3.149		Crippen Method
mcvol	204.820	ml/mol	McGowan Method
rinpol	2050.00		NIST Webbook
rinpol	2050.00		NIST Webbook
rinpol	2050.00		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=R64489&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