4-Quinazolone, 3-ethyl-2-pentyl

Inchi: InChI=1S/C15H20N2O/c1-3-5-6-11-14-16-13-10-8-7-9-12(13)15(18)17(14)4-2/h7-10H,3-
InchiKey: OWILBUJXZJTFDN-UHFFFAOYSA-N
Formula: C15H20N2O
SMILES: CCCCCc1nc2ccccc2c(=O)n1CC
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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64582&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