4-Quinazolone, 3-butyl-2-ethyl

Inchi: InChI=1S/C14H18N2O/c1-3-5-10-16-13(4-2)15-12-9-7-6-8-11(12)14(16)17/h6-9H,3-5,10
InchiKey: QEXSSMRUAXKFHN-UHFFFAOYSA-N
Formula: C14H18N2O
SMILES: CCCCn1c(CC)nc2ccccc2c1=O
Mol. weight [g/mol]: 230.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	2.759		Crippen Method
mcvol	190.730	ml/mol	McGowan Method
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook
rinpol	1961.00		NIST Webbook

Sources

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=R64550&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices