

4-Quinazolone, 2-butyl-3-ethyl

Inchi: InChI=1S/C14H18N2O/c1-3-5-10-13-15-12-9-7-6-8-11(12)14(17)16(13)4-2/h6-9H,3-5,10H
InchiKey: JZZQGMWEIMNCIG-UHFFFAOYSA-N
Formula: C14H18N2O
SMILES: CCCCc1nc2ccccc2c(=O)n1CC
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	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook
rinpol	1962.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R64457&Units=SI>
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>

Legend

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

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