

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,3-5,10H
InchiKey: QEXSSMRUAXKFHN-UHFFFAOYSA-N
Formula: C14H18N2O
SMILES: CCCc1c(CC)nc2cccc2c1=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/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/119-869-6/4-Quinazolone-3-butyl-2-ethyl.pdf>

Generated by Cheméo on 2024-04-29 15:34:43.341219477 +0000 UTC m=+16694132.261796804.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.