4-Quinazolone, 2,3-diethyl

Inchi: InChI=1S/C12H14N2O/c1-3-11-13-10-8-6-5-7-9(10)12(15)14(11)4-2/h5-8H,3-4H2,1-2H3
InchiKey: TZZHUPDVQBATRP-UHFFFAOYSA-N
Formula: C12H14N2O
SMILES: CCc1nc2ccccc2c(=O)n1CC
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	1.979		Crippen Method
mcvol	162.550	ml/mol	McGowan Method
rinpol	1805.00		NIST Webbook
rinpol	1805.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64425&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

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