Quinazolin-4-one, 2-methyl-3-propyl

Inchi: InChI=1S/C12H14N2O/c1-3-8-14-9(2)13-11-7-5-4-6-10(11)12(14)15/h4-7H,3,8H2,1-2H3
InchiKey: PNWIKQLQUSBJBJ-UHFFFAOYSA-N
Formula: C12H14N2O
SMILES: CCCn1c(C)nc2ccccc2c1=O
Mol. weight [g/mol]: 202.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	2.115		Crippen Method
mcvol	162.550	ml/mol	McGowan Method
rinpol	1826.00		NIST Webbook
rinpol	1826.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R560137&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.