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

Inchi: InChI=1S/C12H14N2O/c1-3-6-11-13-10-8-5-4-7-9(10)12(15)14(11)2/h4-5,7-8H,3,6H2,1-2
InchiKey: CZEMEOIWUBRVFH-UHFFFAOYSA-N
Formula: C12H14N2O
SMILES: CCCc1nc2ccccc2c(=O)n1C
Mol. weight [g/mol]: 202.26

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.82		Cheméo Relay (1.0)
logp	1.886		Crippen Method
mcvol	162.550	ml/mol	McGowan Method
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
rinpol	1865.00		NIST Webbook
tf	377.90	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64617&Units=SI

Legend

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

tf: Normal melting (fusion) point