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

Inchi: InChI=1S/C13H16N2O/c1-3-9-15-12(4-2)14-11-8-6-5-7-10(11)13(15)16/h5-8H,3-4,9H2,1
InchiKey: ZIMFYUBAVNPVMC-UHFFFAOYSA-N
Formula: C13H16N2O
SMILES: CCCn1c(CC)nc2ccccc2c1=O
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.63		Cheméo Relay (1.0)
logp	2.369		Crippen Method
mcvol	176.640	ml/mol	McGowan Method
rinpol	1873.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tf	368.27	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R64493&Units=SI
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):

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