

4-Quinazolone, 3-propyl

Inchi:	InChI=1S/C11H12N2O/c1-2-7-13-8-12-10-6-4-3-5-9(10)11(13)14/h3-6,8H,2,7H2,1H3
InchiKey:	XUULXKORCSQLNN-UHFFFAOYSA-N
Formula:	C11H12N2O
SMILES:	CCCN1cnc2ccccc2c1=O
Mol. weight [g/mol]:	188.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.14		Crippen Method
logp	1.806		Crippen Method
mcvol	148.460	ml/mol	McGowan Method
rinpol	1740.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R64635&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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