

Cinchoninamide, 2-methyl-

Other names:	2-methylquinoline-4-carboxamide
Inchi:	InChI=1S/C11H10N2O/c1-7-6-9(11(12)14)8-4-2-3-5-10(8)13-7/h2-6H,1H3,(H2,12,14)
InchiKey:	GPTOAZYKFYMYMW-UHFFFAOYSA-N
Formula:	C11H10N2O
SMILES:	<chem>Cc1cc(C(N)=O)c2cccc2n1</chem>
Mol. weight [g/mol]:	186.21
CAS:	15821-13-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.69		Crippen Method
logp	1.642		Crippen Method
mcvol	144.160	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C15821133&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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

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