

2-Quinazolinamine

Other names:	Quinazoline, 2-amino- 2-Aminoquinazoline
Inchi:	InChI=1S/C8H7N3/c9-8-10-5-6-3-1-2-4-7(6)11-8/h1-5H,(H2,9,10,11)
InchiKey:	CZAAKPFIWJXPQT-UHFFFAOYSA-N
Formula:	C8H7N3
SMILES:	<chem>Nc1ncc2ccccc2n1</chem>
Mol. weight [g/mol]:	145.16
CAS:	1687-51-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.44		Crippen Method
logp	1.212		Crippen Method
mcvol	110.300	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1687510&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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