

4(1H)-Quinazolinone

Other names:	4(3H)-Quinazolinone 4-Hydroxyquinazoline 4-Oxoquinazoline 4-Quinazolinol 4-Quinazolinone 4-Quinazolone Quinazolone, 4- 4(3H)-Quinazolone NSC 5863 Quinazolin-4-one quinazolin-4(1H)-one
Inchi:	InChI=1S/C8H6N2O/c11-8-6-3-1-2-4-7(6)9-5-10-8/h1-5H,(H,9,10,11)
InchiKey:	QMNUDYFKZYBWQX-UHFFFAOYSA-N
Formula:	C8H6N2O
SMILES:	O=c1nc[nH]c2ccccc12
Mol. weight [g/mol]:	146.15
CAS:	491-36-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.68		Crippen Method
logp	0.441		Crippen Method
mcvol	106.190	ml/mol	McGowan Method
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook
rinpol	1733.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C491361&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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