4(1H)-Quinazolinone, 2-methyl-

Other names:	2-Methyl-4-quinazolinone
	2-Methyl-4(3H)-quinazolinone
	2-Methylquinazolone
	2-Methyl-4-quinazolone
	4-Quinazolinol, 2-methyl-
	4(3H)-Quinazolinone, 2-methyl-
	4-Quinazolone, 2-methyl
	2-methylquinazolin-4(1H)-one
Inchi:	InChI=1S/C9H8N2O/c1-6-10-8-5-3-2-4-7(8)9(12)11-6/h2-5H,1H3,(H,10,11,12)
InchiKey:	FIEYHAAMDAPVCH-UHFFFAOYSA-N
Formula:	C9H8N2O
SMILES:	Cc1nc(=O)c2ccccc2[nH]1
Mol. weight [g/mol]:	160.17
CAS:	1769-24-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.16		Crippen Method
logp	0.750		Crippen Method
mcvol	120.280	ml/mol	McGowan Method
rinpol	1736.00		NIST Webbook
rinpol	1736.00		NIST Webbook
rinpol	1736.00		NIST Webbook
ripol	2085.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1769240&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Polar retention indices