4(1H)-Quinolinone, 1-methyl-

Other names:	Echinopsin
	Echinopsine
	N-Methyl-4-quinolone
	1-Methyl-4(1H)-quinolone
	1-Methyl-4-quinolone
	4(1H)-Quinolone, 1-methyl-
	1,4-Dihydro-1-methyl-4-oxoquinoline
	1-Methyl-4(1H)-quinolinone
	Ekhinopsin
	N-Methylquinolin-4-one
	N-Methyl-«gamma»-quinolinone
	1-Methyl-4-quinolinone
Inchi:	InChI=1S/C10H9NO/c1-11-7-6-10(12)8-4-2-3-5-9(8)11/h2-7H,1H3
InchiKey:	CSJAXRKDCCWCSJ-UHFFFAOYSA-N
Formula:	C10H9NO
SMILES:	Cn1ccc(=O)c2ccccc21
Mol. weight [g/mol]:	159.18
CAS:	83-54-5

Physical Properties

Property code	Value	Unit	Source
ie	7.95	eV	NIST Webbook
log10ws	-3.99		Crippen Method
logp	1.538		Crippen Method
mcvol	124.390	ml/mol	McGowan Method

Sources

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=C83545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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