

2(1H)-Quinolinone

Other names:	Carbostyryl «alpha»-Hydroxyquinoline «alpha»-Quinolone o-Aminocinnamic acid lactam 2(1H)-Quinolone 2-Hydroxyquinoline 2-Quinolinol 1H-Quinolin-2-one 2-Quinolinone 2-Quinolone NSC 156783
Inchi:	InChI=1S/C9H7NO/c11-9-6-5-7-3-1-2-4-8(7)10-9/h1-6H,(H,10,11)
InchiKey:	LISFMEBWQUVKPJ-UHFFFAOYSA-N
Formula:	C9H7NO
SMILES:	<chem>O=c1ccc2ccccc2[nH]1</chem>
Mol. weight [g/mol]:	145.16
CAS:	493-62-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.92		Crippen Method
logp	1.046		Crippen Method
mcvol	110.300	ml/mol	McGowan Method
rmpol	1752.00		NIST Webbook
rmpol	293.97		NIST Webbook

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=C493629&Units=SI

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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