

Hydroxymethyl-methaqualon

Other names:	2-(Hydroxymethyl)-3-(2-methylphenyl)-4(3H)-quinazolinone Methaqualone, (2-hydroxymethyl)- 2-Hydroxymethaqualone 4(3H)-Quinazolinone, 2-(hydroxymethyl)-3-o-tolyl- Methaqualone M (2-hydroxymethyl)
Inchi:	InChI=1S/C16H14N2O2/c1-11-6-2-5-9-14(11)18-15(10-19)17-13-8-4-3-7-12(13)16(18)20
InchiKey:	CNRIAQQRQYWDQL-UHFFFAOYSA-N
Formula:	C16H14N2O2
SMILES:	<chem>Cc1cccc1-n1c(CO)nc2cccc2c1=O</chem>
Mol. weight [g/mol]:	266.29
CAS:	5060-49-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.73		Crippen Method
logp	2.186		Crippen Method
mcvol	201.020	ml/mol	McGowan Method
rinsol	2440.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5060491&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

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<https://www.chemeo.com/cid/56-053-1/Hydroxymethyl-methaqualon.pdf>

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