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: Cc1ccccc1-n1c(CO)nc2ccccc2c1=O
Mol. weight [g/mol]: 266.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Cheméo Relay (1.0)
logp	2.186		Crippen Method
mcvol	201.020	ml/mol	McGowan Method
rinpol	2440.00		NIST Webbook
tf	422.31	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5060491&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
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
tf:	Normal melting (fusion) point