Methaqualone

Other names:

(+/-)-Methaqualone
2-Methyl-3-(2-methylphenyl)-4(3H)-quinazolinone
2-Methyl-3-(2-methylphenyl)-4-quinazolinone
2-Methyl-3-(2-tolyl)quinazol-4-one
2-Methyl-3-(o-tolyl)-3,4-dihydro-4-quinazolinone
2-Methyl-3-o-tolyl-4(3H)-chinazolinon
2-Methyl-3-o-tolyl-4(3H)-chinazolone
2-Methyl-3-o-tolyl-4(3H)-quinazolinone
2-Methyl-3-o-tolyl-4-quinazolone
2-Methyl-3-o-tolylquinazolin-4-one
2-Methyl-3-tolyl-4-oxybensdiazine
3,4-Dihydro-2-methyl-4-oxo-3-o-tolylquinazoline
4(3H)-Quinazolinone, 2-methyl-3-(2-methylphenyl)-
4(3H)-Quinazolinone, 2-methyl-3-o-tolyl-
Aqual
CI 705
CN 38703
Cateudyl
Citexal
Dormigoa
Dormigoa-Schlafmittel
Dormogen
Dormutil
Dorsedin
Fadormir
Holodorm
Hyminal
Hypcol
Hypocol
Hyptor
Hyptor base
Ipnofil
MAOA
MTQ
Melsed
Melsedin base
Melsomin
Mequin
Metachalon
Metakvalon

Metaqualon
Methaqualon
Methaqualoneinone
Methased
Metolquizolone
Mollinox
Motolon
Mozambin
Nethaqualone
Nobedorm
Noctilene
Normi-nox
Omnyl
Optinoxan
Orthonal
Ortonal
Parest
Parminal
Pro-dorm
QZ 2
Qu.lovin.a.lovin.alude
Qua.hivin.a.hivin.lude
Quaalude
R-148
RIC 272
Revonal
Rorer 148
Rorer 714
Roulone
Rouqualone
Sindesvel
Somberol
Somnafac
Somnomed
Sonal
Sopor
Soverin
TR 495
Torinal
Tuazol
Tuazole
Tuazolone

Inchi: InChI=1S/C16H14N2O/c1-11-7-3-6-10-15(11)18-12(2)17-14-9-5-4-8-13(14)16(18)19/h3-

InchiKey: JEYCTXHKTXCGPB-UHFFFAOYSA-N
Formula: C16H14N2O
SMILES: Cc1ccccc1-n1c(C)nc2ccccc2c1=O
Mol. weight [g/mol]: 250.30
CAS: 72-44-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Aqueous Solubility Prediction Method
log10ws	-2.92		Estimated Solubility Method
logp	3.003		Crippen Method
mcvol	195.150	ml/mol	McGowan Method
rinpol	2135.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2129.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2144.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2127.00		NIST Webbook
rinpol	2127.00		NIST Webbook
rinpol	2162.00		NIST Webbook
rinpol	2155.00		NIST Webbook
rinpol	2142.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2094.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2117.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2133.00		NIST Webbook
rinpol	2103.00		NIST Webbook
rinpol	2125.00		NIST Webbook

rinpol	2135.00		NIST Webbook
rinpol	2152.00		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2118.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2132.00		NIST Webbook
rinpol	2139.00		NIST Webbook
rinpol	2153.00		NIST Webbook
rinpol	2109.00		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2096.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2117.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2165.00		NIST Webbook
rinpol	2123.00		NIST Webbook
rinpol	2123.00		NIST Webbook
rinpol	2130.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2139.00		NIST Webbook
rinpol	2180.00		NIST Webbook
rinpol	2125.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2105.00		NIST Webbook
ripol	3227.00		NIST Webbook
tf	389.65	K	Aqueous Solubility Prediction Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C72446&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
ripol:	Polar retention indices
tf:	Normal melting (fusion) point