2-Formyl-2-desmethyl-methaqualone

Other names: 2-Quinazolinecarboxaldehyde, 3,4-dihydro-3-(2-methylphenyl)-4-oxo-
Methaqualone M (2-formyl)
Inchi: InChI=1S/C16H12N2O2/c1-11-6-2-5-9-14(11)18-15(10-19)17-13-8-4-3-7-12(13)16(18)20
InchiKey: ZKMDXGXNOKMRKT-UHFFFAOYSA-N
Formula: C16H12N2O2
SMILES: Cc1ccccc1-n1c(C=O)nc2ccccc2c1=O
Mol. weight [g/mol]: 264.28
CAS: 131147-51-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	2.507		Crippen Method
mcvol	196.720	ml/mol	McGowan Method
rinpol	2240.00		NIST Webbook
rinpol	2240.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C131147518&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