3,3-Diisopentenyl-N-methyl-2,4-quinoldione

Inchi: InChI=1S/C20H25NO2/c1-14(2)10-12-20(13-11-15(3)4)18(22)16-8-6-7-9-17(16)21(5)19(
InchiKey: DPDOQGICSCTEJS-UHFFFAOYSA-N
Formula: C20H25NO2
SMILES: CC(C)=CCC1(CC=C(C)C)C(=O)c2ccccc2N(C)C1=O
Mol. weight [g/mol]: 311.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.36		Crippen Method
logp	4.545		Crippen Method
mcvol	262.560	ml/mol	McGowan Method
rinpol	2151.00		NIST Webbook
rinpol	2151.00		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=R405377&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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